TST Review
October 30-31, 2017
### Agenda for TST Site Visit October 30 and 31, 2017

**Monday October 30, 2017**

<table>
<thead>
<tr>
<th>Time</th>
<th>Activity</th>
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<tbody>
<tr>
<td>7:30</td>
<td>Van arriving University Hilton for pickup</td>
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<tr>
<td>7:45</td>
<td>Van leaving University Hilton</td>
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<tr>
<td>8:00-8:45</td>
<td>Full Breakfast (Review team caucus)</td>
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<tr>
<td>8:50-10:00</td>
<td>T1 - CCMT Overview and Integration (Jackson/Bala)</td>
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<tr>
<td>10:00-10:30</td>
<td>T2 – Full System Simulations (Bertrand Rollin)</td>
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<td>10:30-10:45</td>
<td>Coffee break</td>
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<tr>
<td>10:45-11:30</td>
<td>T3 – CMT-nek (Jason Hackl/David Zwick)</td>
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<tr>
<td>11:30-12:00</td>
<td>T4 – ASU Experiments (Blair Johnson)</td>
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<tr>
<td>12:00-1:15</td>
<td>Lunch</td>
</tr>
<tr>
<td>1:15-1:45</td>
<td>T5 – Eglin Experiments (Angela Diggs)</td>
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<tr>
<td>1:45-2:30</td>
<td>T6 - UB (Chanyoung Park; Rafi Haftka; Nam-ho Kim)</td>
</tr>
<tr>
<td>2:30-3:15</td>
<td>T7 - CS (Sanjay Ranka)</td>
</tr>
<tr>
<td>3:15-3:30</td>
<td>Coffee break</td>
</tr>
<tr>
<td>3:30-4:15</td>
<td>T8 - Exascale (Herman Lam/Greg Stitt)</td>
</tr>
<tr>
<td>4:15-4:30</td>
<td>T9 - Internship presentations by Paul Crittenden, Mohamed Gadou, Trokon Johnson, Yash Mehta</td>
</tr>
<tr>
<td>4:30-5:30</td>
<td>Social with Students/Posters (NEB Main Lobby)</td>
</tr>
<tr>
<td>5:30</td>
<td>Transportation to University Hilton by CCMT Faculty</td>
</tr>
<tr>
<td>6:00-7:30</td>
<td>Dinner at the University Hilton, hosted by CCMT Faculty</td>
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</tbody>
</table>
Tuesday October 31, 2017

8:00   Van pickup at University Hilton
8:15-9:00  Continental Breakfast
9:00-10:30 Student Presentations
   T10 – EOS Surrogate Modeling (Fred Ouellet)
   T11 – UQ & Instabilities (Giselle Fernandez)
   T12 – PIEP Modeling (Chandler Moore)
   T13 – Microscale Shock-Contact Modeling (Brandon Osborne)
   T14 – BE of CMT-nek (Sai Chenna)

10:30-11:30 Discussions between TST and CCMT PIs

11:30  Box Lunch; Transportation to hotel and/or airport as needed
# TST Review October 30-31, 2017 Attendee List

## Faculty

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td>S. Balachandar “Bala”</td>
<td>University of Florida</td>
<td><a href="mailto:bala1s@ufl.edu">bala1s@ufl.edu</a></td>
</tr>
<tr>
<td>Rafi Haftka</td>
<td>University of Florida</td>
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</tr>
<tr>
<td>Nam-Ho Kim</td>
<td>University of Florida</td>
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</tr>
<tr>
<td>Herman Lam</td>
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<tr>
<td>Sanjay Ranka</td>
<td>University of Florida</td>
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</tr>
<tr>
<td>Greg Stitt</td>
<td>University of Florida</td>
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</tr>
<tr>
<td>Tom Jackson</td>
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<td><a href="mailto:tlj@ufl.edu">tlj@ufl.edu</a></td>
</tr>
<tr>
<td>Siddharth Thakur “ST”</td>
<td>University of Florida</td>
<td><a href="mailto:sst@ufl.edu">sst@ufl.edu</a></td>
</tr>
<tr>
<td>Bertrand Rollin</td>
<td>Embry-Riddle</td>
<td><a href="mailto:rollinb@erau.edu">rollinb@erau.edu</a></td>
</tr>
<tr>
<td>Angela Diggs</td>
<td>Eglin Air Force Base</td>
<td><a href="mailto:angela.diggs.1@us.af.mil">angela.diggs.1@us.af.mil</a></td>
</tr>
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## Review Team

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Email</th>
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<tr>
<td>Abhinav Bhatele</td>
<td>LLNL</td>
<td><a href="mailto:bhatele1@llnl.gov">bhatele1@llnl.gov</a></td>
</tr>
<tr>
<td>David Daniel</td>
<td>LANL</td>
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</tr>
<tr>
<td>Maya Gokhale</td>
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<tr>
<td>Sam Schofield (Chair)</td>
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</tr>
<tr>
<td>Mark Schraad</td>
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<tr>
<td>Justin Wagner</td>
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<td><a href="mailto:jwagner@sandia.gov">jwagner@sandia.gov</a></td>
</tr>
<tr>
<td>Greg Weirs</td>
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<td><a href="mailto:vgweirs@sandia.gov">vgweirs@sandia.gov</a></td>
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## Others

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<tr>
<td>Bob Voigt</td>
<td>Leidos/NESD</td>
<td><a href="mailto:rvoigt@krellinst.org">rvoigt@krellinst.org</a></td>
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## Research Staff

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<tr>
<td>Tania Banerjee</td>
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## Center for Compressible Multiphase Turbulence

### Students

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<tr>
<th>Name</th>
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<tr>
<td>Ryan Blanchard</td>
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<tr>
<td>Heather Zunino</td>
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<tr>
<td>David Zwick</td>
<td></td>
<td><a href="mailto:dpzwick@ufl.edu">dpzwick@ufl.edu</a></td>
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### Administration Staff

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<thead>
<tr>
<th>Name</th>
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<tr>
<td>Hollie Starr</td>
<td></td>
<td><a href="mailto:hstarr@ufl.edu">hstarr@ufl.edu</a></td>
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### Financial Staff

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<th>Email</th>
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<tr>
<td>Melanie DeProspero</td>
<td></td>
<td><a href="mailto:mel7703@ufl.edu">mel7703@ufl.edu</a></td>
</tr>
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</table>
CCMT Overview and Integration

T.L. Jackson
S. Balachandar

TST Meeting Agenda

Monday
- T1 - Overview and Integration (Jackson & Balachandar)
- T2 – Full System Simulations (Bertrand Rollin)
- Coffee Break
- T3 - CMT-nek (Jason Hackl & David Zwick)
- T4 - ASU Experiments (Blair Johnson)
- Lunch
- T5 - Eglin Experiments (Angela Diggs)
- T6 - Uncertainty Budget (Chanyoung Park, Rafi Haftka, Nam-Ho Kim)
- T7 - CS (Sanjay Ranka)
- Coffee Break
- T8 - Exascale (Herman Lam & Greg Stitt)
- T9 - Internship presentations
- Social with Students/Posters (NEB Main Lobby)
- Dinner at University Hilton with CCMT Faculty and Staff

Tuesday
- Student Talks (5)
- Discussions between TST and CCMT PIs
- Lunch and transportation to airport
## Leadership

### Physics and Code Development

- S. (Bala) Balachandar
- Siddharth Thakur (ST)
- Thomas Jackson
- Paul Fischer
- Ju Zhang
- Bertrand Rollin
- Stanley Ling
- Raphael Haftka
- Nam-Ho Kim

### UQ and V&V

- Ronald Adrian
- Charles Jenkins
- Donald Littrell
- Sanjay Ranka
- Herman Lam
- Gregory Stitt
- Scott Parker

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## Research Staff & Senior PhD Students

- Tania Banerjee
- Angela Diggs (Eglin AFB)
- Jason Hackl
- Blair Johnson (ASU)
- Chanyoung Park
- Carlo Pascoe
- Nalini Kumar

*UF members in red*
### Internship Program - Completed

- **Heather Zunino**  
  LANL  
  May-Aug, 2014  
  Dr. Kathy Prestridge

- **Kevin Cheng**  
  LLNL  
  May-Aug, 2014  
  Dr. Maya Gokhale

- **Nalini Kumar**  
  Sandia  
  March-Aug, 2015  
  Dr. James Ang

- **Christopher Hajas**  
  LLNL  
  May-Aug, 2015  
  Dr. Maya Gokhale

- **Christopher Neal**  
  LLNL  
  June-Aug, 2015  
  Dr. Kambiz Salari

- **Carlo Pascoe**  
  LLNL  
  June-Aug, 2015  
  Dr. Maya Gokhale

- **Giselle Fernandez**  
  Sandia  
  Oct-Dec, 2015  
  Drs. Gregory Weirs & Vincent Mousseau

- **Justin Mathew**  
  LANL  
  May-Aug, 2015  
  Dr. Nick Hengartner

- **David Zwick**  
  Sandia  
  May-Aug, 2016  
  Drs. John Pott & Kevin Ruggirello
### Internship Program - Completed

<table>
<thead>
<tr>
<th>Intern Name</th>
<th>Institution</th>
<th>Term</th>
<th>Mentors</th>
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<tbody>
<tr>
<td>Goran Marjanovic</td>
<td>Sandia</td>
<td>Aug-Nov, 2016</td>
<td>Drs. Paul Crozier &amp; Stefan Domino</td>
</tr>
<tr>
<td>Georges Akiki</td>
<td>LANL</td>
<td>May-Aug, 2016</td>
<td>Dr. Marianne Francois</td>
</tr>
<tr>
<td>Paul Crittenden</td>
<td>LLNL</td>
<td>Spring, 2017</td>
<td>Drs. Kambiz Salari &amp; Sam Schofield</td>
</tr>
<tr>
<td>Mohamed Gadou</td>
<td>LANL</td>
<td>Summer, 2017</td>
<td>Dr. Galen Shipman</td>
</tr>
<tr>
<td>Trokon Johnson</td>
<td>LANL</td>
<td>Summer, 2017</td>
<td>Drs. Cristina Garcia-Cardona, Brendt Wohlb, Erik West</td>
</tr>
<tr>
<td>Yash Mehta</td>
<td>LLNL</td>
<td>Summer, 2017</td>
<td>Dr. Kambiz Salari</td>
</tr>
<tr>
<td>Kyle Hughes</td>
<td>LANL</td>
<td>Fall, 2017</td>
<td>Dr. Kathy Prestridge</td>
</tr>
</tbody>
</table>

### Internship Program – Not Yet Planned

- Brad Durant, PhD (MAE, Physics and UQ)
- Joshua Garno, PhD (MAE, Physics and UQ)
- Brandon Osborne, PhD (MAE, Physics)
- Fred Ouellet, PhD (MAE, Physics and UQ)
- Chandler Moore, PhD (MAE, Physics) (NSF Fellowship)
### Graduated Students & Postdocs

- Kevin Cheng, MS (2014), Dr. Alan George, ECE
- Hugh Miles, BS (2015), Dr. Greg Stitt, ECE
- Chris Hajas, MS (2015), Dr. Herman Lam, ECE
- Angela Diggs, PhD (2015), Dr. S. Balachandar, MAE
  - Currently employed at Eglin AFB and working with center
- Bertrand Rollin, Postdoc in thru August 2014
  - Assistant Professor, Embry Riddle, Daytona Beach FL
- Mrugesh Shringarpure, Postdoc in thru January 2016
  - Research Engineer, ExxonMobil, Houston TX
- Subbu Annamalai, PhD (2015), Dr. S. Balachandar, MAE; Postdoc in thru March 2017
  - Senior Systems Engineer, Optym, Gainesville FL
- Georges Akiki, PhD (2016), Dr. S. Balachandar, MAE; Postdoc thru March 2017
  - Postdoctoral Associate, LANL
- Nalini Kumar, PhD (August, 2017), Dr. H. Lam, ECE
  - Intel, Santa Clara CA

### Additional Information

- Additional Graduate Program Announcements
  - David Zwick – NSF Fellowship Graduate Program (Aug 2016)
  - Georges Akiki - MAE Best Dissertation Award (TSFD; May 2017)
  - Chandler Moore – NSF Fellowship Graduate Program (Aug 2017)

- Other metrics (Y1 – Y3)
  - Publications: 85
  - Presentations: 69

- Deep Dive Workshops
  - Exascale & CS Issues, Feb 3-4, 2015, University of Florida
  - Multiphase Physics, Oct 13-14, 2016, Tampa FL

- APS Special Focus on UQ (July, 2017) – Jackson, Najjar, Najm

- Center Webpage
  - http://www.eng.ufl.edu/ccmt/
Educational Programs

- Institute for Computational Science (ICE)
- Course in Verification, Validation and Uncertainty Quantification taught every third semester (N. Kim, R. Haftka)
- Yearly a specialized course for HPC for computational scientists (as part of the Computational Engineering Certificate) (S. Ranka)
- Fall, 2016 – new graduate course on multiphase flows (S. Balachandar)
- Discusses exascale challenges and the NGEE work in the reconfigurable computing course (EEL5721/4720) and digital design (EEL4712) (H. Lam, G. Stitt)
- Uses the CCMT center as a motivational example in Introduction to Electrical and Computer Engineering (EEL3000) (H. Lam, G. Stitt)
- EEL6763 (Parallel Computer Architecture) (A. George/Ian Troxel)

Management: Tasks and Teams

*The Center is organized by physics-based tasks and cross-cutting teams, rather than by faculty and their research groups*

<table>
<thead>
<tr>
<th>Hour time slots</th>
<th>Exascale</th>
<th>CMT-nek</th>
<th>CS</th>
<th>Micro</th>
<th>Macro/Meso</th>
<th>UQ</th>
<th>Exp</th>
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<td>UQ</td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Weekly interactions (black); Regular interactions (red)
- Teams include students, staff, and faculty
- All staff and large number of graduate students located on 2nd floor of PS&T Building
- Construction in PS&T Building to add 6 new office spaces for students
- All meetings held in PS&T Building
Outline

- Background
- Scope of the center
- V&V and UQ workflow
- Y4 accomplishments
- Integration and timeline
Demonstration Problem

Prediction Metrics

- PM-1: Blast Wave Location
- PM-2: Particle Front Location
- PM-3: Number of Instability Waves
- PM-4: Amplitude of Instability Waves
**Sequence of Events**

- **Detonation phase**
  - Metal particles
  - Explosive material
  - Hot, dense, high pr gas
  - Shock wave

- **Dispersion phase**

- **Compaction/collision phase**

**Physical Models – Sources of Error**

- **T1**: Detonation model
- **T2**: Multiphase turbulence model
- **T3**: Thermodynamic & transport model
- **T4**: Interaction model
- **T5**: Compaction model
- **T6**: Point particle force model
- **T7**: Point particle heat transfer model
- **T8**: Deformation model
Multiphysics Scope (From Site Visit)

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities
  - Gas-particle coupling
  - Self-assembly of explosive-driven particles

- Will avoid the following complications
  - Free-shear and wall turbulence (stay away from boundaries)
  - Detonation physics (use simple, well-studied explosives)
  - Fragmentation or atomization physics (avoid casing, liquids)
  - Reactive physics (use non-reactive metal particles)
**Sources of Errors & Uncertainties**

- T1: Detonation modeling
- T2: Multiphase turbulence modeling
- T3: Thermodynamics & transport properties
- T4: Particle-particle interaction modeling
- T5: Compaction modeling
- T6: Force coupling modeling
- T7: Thermal coupling modeling
- T8: Particle deformation and other complex physics
- T9: Discretization and numerical approximation errors
- T10: Experimental and measurement errors & uncertainties

**Key Focus**
- Advance state-of-the-art
  - Multiphase turbulence
  - Force coupling model

**Amendment to Scope**

- Our focus will be on
  - Turbulence at the rapidly expanding material front
  - Rayleigh-Taylor (RT) and Richtmeyer-Meshkov (RM) instabilities
  - Gas-particle coupling
  - Self-assembly of explosive-driven particles

- We have added an intermediate configuration that minimizes
  - Compaction effect and associated modeling (T5)

- Revised plan includes
  - Mesoscale and demonstration experiments with lower $\phi$
  - Use hollow spheres (thin glass beads)
Uncertainty Budget – Overall Plan

- T2 – Turbulence modeling
- T5 – Compaction modeling
- T4 – Particle interaction modeling
- T6 – Force coupling modeling

4 Micro/Meso Campaigns & Target Models

- Sandia shock-tube
  - T6: Force coupling and T4: Particle-particle interaction
- ASU expansion fan
  - T2: Multiphase turbulence and T4: Particle-particle interaction
- Eglin microscale
  - T6: Force coupling
- Eglin mesoscale gas-gun
  - T5: Compaction
- Demonstration problem
  - Yearly hero run
Uncertainty Budget Workflow

Experiments → Experimental input → Simulations

Input uncertainty → Target model improvement

Large? → Target model error → Computed Metrics

Measured Metrics → Target model error

Empty Success (Small error, but Large Uncertainty) → Useful Failure

Control Parameter

Uncertainty Budget Workflow

Experiments → Experimental input → Simulations

Input uncertainty → Target model improvement

Large? → Target model error → Computed Metrics

Measured Metrics → Target model error

Uncertainty/error reduction → Large? → Uncertainty/error reduction

Sampling uncertainty
Measurement uncertainty
Measurement processing error

Uncertainty
Error

Propagated uncertainty
Stochastic variability
Discretization error
Neglected feature/physics
**UB Workflow - Experiment Worksheet**

- **Experimental input**
  - Shock properties, particle properties, curtain properties, ...

- **Input uncertainty**
  - Quantified uncertainties in all the above

- **Prediction metrics**
  - PM1: Shock position, PM2: Upstream and downstream curtain

- **Uncertainty & error quantification (UQ)**
  - Error in PM1 and PM2 obtained from Schlieren
  - Error in X-ray image particle volume fraction

- **Uncertainty & error reduction (UR)**
  - Perform new experiments without spanwise gap
  - Improved measurement to reduce volume fraction uncertainty

---

**Hierarchical Error Estimation and UQ**

![Diagram showing the relationship between VVUU framework, target model, and various simulations and experiments at different scales (Eglin Macroscale Experiments, Eglin Macroscale Simulations, Eglin Microscale Experiments, SNL Shocktube Experiments, ASU Vertical Shocktube Exp., ASU Mesoscale Simulation, SNL Mesoscale Simulations, Eglin Gas gun Experiments).]
Other Simulation Campaigns

- Microscale simulations of shock+contact over structured and random array of particles
  - Testing and improvement of force coupling (T6)
- Mesoscale simulations of turbulent multiphase jet/plume
  - Testing and improvement of multiphase LES (T2)
- Mesoscale simulations of sedimentation
  - Testing and improvement of particle-particle interaction model (T4)
- Mesoscale simulations of controlled instability
  - Evaluation of PM3 and PM4

Y4 Key Accomplishments

- Tight integration
- Empower students and staff
- PIEP model
- CMT-nek \( (O(10^6) \text{ core simulations}) \)
- Culture of UQ integration
- BE framework and FPGA
- Dynamic load balancing
## Y4 Highlights

1. Macroscale – Hero Run
2. Blastpad & other validation experiments
3. CMT-nek development and transition
4. Mesoscale – CMT-nek simulation of expansion fan
5. Microscale – Shock + Contact
6. UQ workflow
7. Design space exploration with Behavioral Emulation
8. Dynamic load balancing of Euler-Lagrange

## 1: Demonstration Problem (Macroscale)

**Goal**
- Yearly perform the largest possible simulations of the demonstration problem and identify improvements to be made in predictive capability

**Year 4**
- Used existing code to perform largescale simulations of the demonstration problem
- Qualitative comparison against experimental data of Frost (PM1 & PM2)
- Develop capabilities for the hero runs: real gas EOS, reactive burn, collision modeling

**Presentation**
- Bertrand Rollin

![3-D demonstration Simulations](image)
2: Blastpad Experiments

Goals
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

Year 4
- Blast pad experiments at Eglin AFB
- Detailed instrumentation for validation
- Simulation informed experiments
- Integrated UQ

Presentation
- Angela Diggs, Bertrand Rollin

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explosive length [mm]</td>
<td>AFRL measurement</td>
</tr>
<tr>
<td>Explosive diameter [mm]</td>
<td>AFRL measurement at 5 locations</td>
</tr>
<tr>
<td>Explosive density [kg/m³]</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Explosive quality</td>
<td>AFRL X-ray</td>
</tr>
<tr>
<td>Particle diameter [mm]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle density [kg/m³]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle volume fraction</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Ambient pressure [kPa]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Ambient temperature [°C]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Probe locations [m]</td>
<td>CCMT measurement</td>
</tr>
</tbody>
</table>

SEM of single steel particle at 1000x zoom.  
SEM of several steel particles at 100x zoom.
2: Mesoscale Experiments

Goals
- Obtain validation-quality experimental measurements of the demonstration problem
- Validation-quality experiments at micro and mesoscales
- Perform shock-tube track micro- and mesoscale experiments

Year 4
- Expansion fan experiments at ASU
- Detailed instrumentation for validation
- Simulation informed experiments
- Integrated UQ

Presentation
- Blair Johnson (ASU)

3: CMT-nek Development

Goals
- Co-design an exascale code (CMT-nek) for compressible multiphase turbulence
- Perform micro, meso and demonstration-scale simulations
- Develop & incorporate energy and thermal efficient exascale algorithms

Year 4
- Developed and released microscale version of CMT-nek for microscale simulations
- Developed and released mesoscale version of CMT-nek for mesoscale simulations
- Shock capturing with EVM
- CMT-nek in nek5000 repository

Presentation
- Jason Hackl and David Zwick
3. CMT-nek

- Capabilities
  - Viscous compressible N-S solver
  - DG spectral element (rigorous conservation)
  - Shock capturing with EVM
  - Spectrally accurate Lagrangian particle solver
  - 4-way coupling (Soft-sphere DEM, PIEP)
  - Scalable to \( O(10^6) \) cores and more

- Class of problems
  - Incompressible (Nek-5000) & compressible single phase
  - Incompressible & compressible dilute point-particle multiphase
  - Incompressible & compressible dense multiphase

4: Mesoscale Simulations

Goal
- Perform a hierarchy of mesoscale simulations to allow rigorous validation, uncertainty quantification and propagation to the demonstration problem

Year 4
- 2-way coupled simulation with CMT-nek
- Mesoscale simulations of expansion fan over a bed of particles
- 4-way coupled simulations with and without PIEP
- Bundled simulations for UQ

Presentation
- David Zwick
5: Microscale Simulations

Goals
- Perform a hierarchy of microscale simulations at conditions of relevance
- Develop extended point-particle models
- Rigorous validation, uncertainty quantification and propagation

Year 4
- Shock propagation over a structured array
- Shock propagation over a random array
- Shock + Contact + particles
- Shock over deformable particles

Presentation
- Brandon Osborne

5: Extended Point Particle Model

ϕ = 44%, Re = 20, N = 459

<table>
<thead>
<tr>
<th>ϕ</th>
<th>Re</th>
<th>Drag</th>
<th>Lift</th>
<th>Torque</th>
<th>Drag</th>
<th>Lift</th>
<th>Torque</th>
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<td>0.67</td>
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<td>0.35</td>
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<td>0.44</td>
<td>0.60</td>
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<td>0.2</td>
<td>16</td>
<td>0.38</td>
<td>0.34</td>
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<tr>
<td>0.2</td>
<td>80</td>
<td>0.50</td>
<td>0.48</td>
<td>0.72</td>
<td>0.62</td>
<td>0.63</td>
<td>0.77</td>
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<tr>
<td>0.45</td>
<td>21</td>
<td>0.01</td>
<td>0.09</td>
<td>0.47</td>
<td>0.55</td>
<td>0.59</td>
<td>0.76</td>
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<tr>
<td>0.45</td>
<td>115</td>
<td>0.21</td>
<td>0.19</td>
<td>0.51</td>
<td>0.63</td>
<td>0.57</td>
<td>0.65</td>
</tr>
</tbody>
</table>
6: UQ Workflow

Goals
- Develop UB as the backbone of the Center
- Unified application of UB for both physics and exascale emulation

Year 4
- Identify main uncertainty sources and quantify their contributions to the model uncertainty of the shock tube simulation
- Reduce uncertainty to focus on model error
- UQ and propagation in the context of exascale emulation
- JWL mixture-EOS surrogate for efficient computation

Presentation
- Rafi Haftka, Chanyoung Park, Giselle Fernandez, Fred Ouellet

7: Exascale Emulation

Goal
- Develop behavioral emulation (BE) methods and tools to support co-design for algorithmic design-space exploration and optimization of key CMT-bone kernels & applications on future Exascale architectures

Year 4
- Enhanced BE methods with network models, interpolation schemes, and benchmarking for CMT-bone AppBEOS
- Performed large-scale experiments on DOE platforms with BE-SST simulator
- Started design space exploration
- Improved throughput and scalability for FPGAs

Presentation
- Herman Lam, Greg Stitt, Sai Chenna
8: Dynamic Load Balancing

Goal
- Derive computationally intensive portions of the CMT-nek code and understand its performance, thermal and energy issues

Year 4
- Carried out extensive investigation of performance and energy issues for CMT-bone
- Hybrid CPU-GPU implementation of CMT-bone and optimization
- Thermal aware optimization
- Dynamic load balancing with particles

Presentation
- Sanjay Ranka

Transition to CMT-nek – Simulation Plan
**Transition to CMT-nek – CCMT Workshop**

**A Boot Camp on CMT-nek**

November 29, 2017

Organizers: Bertrand Rollin, Jason Hackl

---

**Agenda**

- **CMT-nek: Anatomy of the Beast**
  Speaker: Jason Hackl | 12:00 pm – 1:30 pm

- **Lagrangian Particles in CMT-nek**
  Speaker: David Zwick | 1:30 pm – 2:30 pm

- **Running CMT-nek**
  Speakers: Goran Marjanovic and Brad Durant | 2:30 pm – 3:15 pm

- **Post-Processing and visualization in CMT-nek**
  Speakers: David Zwick and Brad Durant | 3:15 pm – 4:00 pm

- **Lesson Learnt from CCMT’s Simulations**
  Speakers: Fred Ouellet and Yash Mehta | 4:00 pm – 5:00 pm

---

**Attendee list**

- Paul Crittenden
- Brad Durant
- Giselle Fernandez
- Joshua Garno
- Jason Hackl
- Rahul Koneru
- Yash Mehta
- Goran Marjanovic
- Chandler Moore
- Fred Ouellet
- Brandon Osborne
- Bertrand Rollin
- Prashanth Sridharan
- David Zwick

---

**Transition to CMT-nek – Timeline**

<table>
<thead>
<tr>
<th>Task</th>
<th>Year4</th>
<th>Year5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NOV</td>
<td>DEC</td>
</tr>
<tr>
<td>Training with CMT-nek</td>
<td>W</td>
<td></td>
</tr>
<tr>
<td>Blastpad Simulation 3D (Hero Run)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Mesoscale Experiment (2D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Mesoscale Experiment (3D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Microscale Experiment (2D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Microscale Experiment (3D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sandia Shock Tube Experiment</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ASU Expansion Fan</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

W Workshop: "A Boot Camp on CMT-nek"
### CMT-nek – Blastpad Hero Runs

<table>
<thead>
<tr>
<th></th>
<th>Hero Run 6</th>
<th>Hero Run 7</th>
<th>Hero Run 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactive burn</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Equation of state</td>
<td>Ideal Gas</td>
<td>JWL</td>
<td>JWL</td>
</tr>
<tr>
<td>Initial Particle volume fraction</td>
<td>5%</td>
<td>10%</td>
<td>60%</td>
</tr>
<tr>
<td>Particle bed perturbation</td>
<td>none</td>
<td>1 mode – (Notched Case)</td>
<td>Random</td>
</tr>
<tr>
<td>No. of computational particles</td>
<td>20B</td>
<td>20B</td>
<td>20B</td>
</tr>
<tr>
<td>No. of Grid Points</td>
<td>1.8B (1,025,000 Spectral Elements, 12x12x12 grid points/element)</td>
<td>1.8B (1,025,000 Spectral Elements, 12x12x12 grid points/element)</td>
<td>14B (8,200,000 Spectral Elements, 12x12x12 grid points/element)</td>
</tr>
<tr>
<td>No. of cores</td>
<td>131K</td>
<td>131K</td>
<td>393,216 (All of Vulcan - DAT)</td>
</tr>
<tr>
<td>Simulation Time</td>
<td>0.5ms</td>
<td>3.0ms</td>
<td>6.0ms</td>
</tr>
</tbody>
</table>

### Hierarchical Error Estimation and UQ

- **VVUU framework**
  - Target model

- **Eglin Macroscale Simulations**
- **Eglin Macroscale Experiments**

- **SNL Mesoscale Simulations**
- **SNL Shocktube Experiments**

- **ASU Vertical Shocktube Exp.**
- **ASU Mesoscale Simulation**

- **Model error estimation and UQ of T6 and T4 will be com by Y4Q4**
  - UQ of the particle curtain model is being carried out
Model error estimation and UQ of T6 (Y5Q2)
- Finished the experiments (Y2Q2)
- Complete interventional UQ of the experiments (Y5Q1)
- Complete microscale simulation (Y5Q1)
- Quantify numerical error (Y4Q4)

Model error estimation and UQ of T2 and T4 will be finished by Y5Q4
- Plan for validating the turbulence model T2 (Y5Q1)
- Complete a simulation with the turbulence model into CMT-nek (Y5Q3)
- Quantify numerical error of the turbulence model (Y5Q4)
- Prepare experiment plan for measuring prediction metrics (Y6Q1)
- Complete the planned experiments (Y6Q2)
- Complete interventional UQ of the experiments (Y6Q3)
Hierarchical Error Estimation and UQ

- Model error estimation and UQ of T5 (Y5Q4)
  - Finished the experiments (Y4Q3)
  - Complete interventional UQ of the experiments (Y5Q1)
  - Complete mesoscale simulation (Y5Q2)
  - Quantify numerical error (Y5Q2)

Prediction error estimation and UQ of demonstration simulation (Y6Q4)
- Complete Eglin Blast pad experiments (Y5Q4)
- Complete interventional UQ of the experiments (Y6Q1)
- Complete lower fidelity simulation(s) for UQ with multi-fidelity surrogate (Y5Q1)
- Quantify numerical error of the lower fidelity simulation (Y5Q1)
- Complete hero simulations (Y5Q4)
- Quantify numerical error of hero simulation (Y5Q4)
Do you have any questions?
Full System Simulations

Bertrand Rollin
Bring predictive capabilities to particle-laden flow simulations under extreme conditions

Outline

- Demonstration Problems
  - Frost's Experiment
  - Eglin's Blastpad Experiment

- Micro and Mesoscale Campaigns
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - SNL's Multiphase Shock Tube
  - ASU Expansion Fan
Physical Models – Sources of Error

T1: Detonation model
- Explosive material
- Hot, dense, high pr gas

T2: Multiphase turbulence model

T3: Thermodynamic & transport model

T4: Collision model
- Shock wave

T5: Compaction model
- Metal particles

T6: Point particle force model

T7: Point particle heat transfer model

T8: Deformation model
- Compaction/collision phase

Dispersion phase

Hero Runs

HR 2
- Features:
  - 30 Million computational cells
  - 5 Million computational particles
  - $r_{\text{max}} = 4.00\text{m}$
  - $t_{\text{max}} = 2.50\text{ms}$
  - 4096 cores

HR 3
- Features:
  - 60 Million computational cells
  - 15 Million computational particles
  - $r_{\text{max}} = 4.00\text{m}$
  - $t_{\text{max}} = 1.40\text{ms}$
  - 5760 cores
**Hero Run: Evolution**

<table>
<thead>
<tr>
<th>Reactive burn</th>
<th>Hero Run 1</th>
<th>Hero Run 2</th>
<th>Hero Run 3</th>
<th>Hero Run 4A</th>
<th>Hero Run 4B</th>
<th>Hero Run 5</th>
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<tr>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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<td>Yes</td>
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<table>
<thead>
<tr>
<th>Equation of state</th>
<th>Ideal Gas</th>
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<th>JWL</th>
<th>JWL</th>
<th>JWL</th>
<th>JWL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Particle volume fraction</td>
<td>5 %</td>
<td>40 % - Frozen</td>
<td>10 % - Frozen</td>
<td>10 % - Frozen</td>
<td>10 % - Frozen</td>
<td>10 % - Frozen</td>
</tr>
<tr>
<td>Particle bed perturbation</td>
<td>none</td>
<td>none</td>
<td>1 mode in azimuthal direction</td>
<td>none</td>
<td>4 mode in azimuthal direction + white noise</td>
<td>none</td>
</tr>
<tr>
<td>No. of computational particles</td>
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<td>5 M</td>
<td>15 M</td>
<td>15 M</td>
<td>15 M</td>
<td>30 M</td>
</tr>
<tr>
<td>No. of elements</td>
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<td>30 M</td>
<td>60 M</td>
<td>60 M</td>
<td>60 M</td>
<td>120 M</td>
</tr>
<tr>
<td>No. of cores</td>
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<td>4096</td>
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<td>5760</td>
<td>5760</td>
<td>16384</td>
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<tr>
<td>Simulation Time</td>
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<td>2.5ms</td>
<td>1.40ms</td>
<td>0.20ms</td>
<td>0.42ms</td>
<td>0.03ms</td>
</tr>
</tbody>
</table>

**Hero Run 3: Reactive Burn Initial Conditions**

Currently running

---

Page 31 of 174
The Jones-Wilkins-Lee (JWL) equations of state are used to predict the pressures of high energy substances and are:

\[
P_{\text{JWL}}(\rho, \epsilon) = A(1 - \frac{\rho}{\rho_0})e^{-R_1\rho} + B(1 - \frac{\rho}{\rho_0})e^{-R_2\rho} + \omega \rho \\
T_{\text{JWL}}(P, \rho) = \left( \frac{1}{\rho} \right) (P - A e^{-R_1\rho} - B e^{-R_2\rho})
\]

where \( V = \frac{\rho}{\rho_0} \) and \( \rho_0, A, B, C, R_1, R_2, \) and \( \omega \) are parameters for the substance.

### Iterative method | One Equation | Multi-fidelity Surrogate
---|---|---
**Advantage** | - Accuracy | - Speed | - Speed
- Problem independent | - Algebraic equation | - Take account of species equation

**Disadvantage** | - May be slow to converge | - Uncertainty and error | - Uncertainty
- Computationally expensive | - JWL + ideal gas case only | - Equation of State specific (problem specific)

➢ “EoS Surrogate Modeling”, Fred Ouellet
Demonstration Problem: Predictions

Particle Front Location (PM-2)

Hero Run 3 – A Closer Look
CCMT

Hero Run 3 – A Closer Look

- Multi-fidelity surrogate model for finding the fastest growing initial perturbation
  M. Giselle Fernandez-Godino

- Hero Run 3

- t=0, k=24
- t=168µs, k=24 and k=48
- t=962µs, k=24 emerging again
- t=480µs, No dominant modes

- Outline

  - Demonstration Problems
    - Frost’s Experiment
    - Eglin’s Blastpad Experiment
  
  - Micro and Mesoscale Campaigns
    - Eglin Microscale Experiments
    - Eglin Mesoscale Experiments
    - SNL’s Multiphase Shock Tube
    - ASU Expansion Fan
AFRL Blastpad Experimental Setup

- **Instrumentation:**
  - 54 pressure probes
  - Momentum traps (instrumented possible)
  - Four high speed video cameras
  - Linear optical transducers

- **Six shots**
  - 2 bare charges
  - 1 charge w/tungsten (notched)
  - 1 charge w/steel (notched)
  - 2 charges w/steel (un-notched)

Locations of 54 pressure transducers (Barreto et al. 2015).

- "Eglin Experiment", Angela Diggs

Blastpad Simulation (Bare charge 1d results)

1D Simulation Details:
- 100,000 cells in radial direction up to 6 m.
- Run using 16 cores up to a time of 4.5 ms
- 1 Equation JWL Model for Composition-B used for EoS
Blastpad Simulation Setup

Preliminary Simulation Details:
- 1 million cells in two dimensions
- To be run on 256 cores using LLNL’s Quartz machine
- Exhaust boundary is an outflow
- Other bottom boundaries are slipwalls
- 4 probes set in locations of experimental sensors
- 40 other probes set in near-charge region

Note: Bare charge setup is shown, particles will be included in parallel runs

Outline

- **Demonstration Problems**
  - Frost’s Experiment
  - Eglin’s Blastpad Experiment

- **Micro and Mesoscale Campaigns**
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - SNL’s Multiphase Shock Tube
  - ASU Expansion Fan
Simulations implement the JWL equation of state and reactive burn initial condition for the explosive.

Plan for Uncertainty Quantification Analysis:
- Vary input parameters of particle density, particle diameter, and explosive mass for batch run (5 x 5 x 5 x 3 simulations) to construct surrogate model.
- Done for all variations of particle configuration.

Current geometry has a solid backwall for the explosive:
- In reality there is a sizable hole in the back of the explosive where the detonator attaches.
- Simulations will compare the effects of including this hole.
Simulation Results

Simulation Details:
- Axisymmetric
- Real gas equation of state (JWL)
- Point-particle model
- Explosive modeled with a reactive burn initial profile
- Time-shifted to align with experimental times
- 1-way coupled (1 Particle)

Outline

- **Demonstration Problems**
  - Frost's Experiment
  - Eglin's Blastpad Experiment

- **Micro and Mesoscale Campaigns**
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - **SNL's Multiphase Shock Tube**
  - ASU Expansion Fan
New Particle Curtain Experiments

Large-Scale Bundle Runs

- Comparison between mesoscale 1D/2D/3D simulations and the new SNL experiments with non-tophat initial particle volume fraction profile
  - Runs for:
    - 5 different Mach numbers: 1.24, 1.40, 1.45, 1.66, 1.92
    - Initial particle volume fraction
    - Random initial particle locations
    - Curtain thickness
  - 625 1D bundle runs with Dakota
  - 135 2D runs
  - 27 3D runs

- "Uncertainty Budget", Chanyoung Park
### 3D Particle Curtain Simulation

- **Features:**
  - 18 Million computational cells
  - 6 Million computational particles
  - 2048 cores

### Shock Tube Results

- Particle fronts are defined as the locations of the trailing and leading 0.5% of particles

  ➢ "Uncertainty Budget", Chanyoung Park
Outline

- **Demonstration Problems**
  - Frost’s Experiment
  - Eglin’s Blastpad Experiment

- **Micro and Mesoscale Campaigns**
  - Eglin Microscale Experiments
  - Eglin Mesoscale Experiments
  - SNL’s Multiphase Shock Tube
  - ASU Expansion Fan

---

ASU Experiment

• Simulations are progressing with CMT-nek
  - “CMT-nek”, Jason Hackl and David Zwick
  - “ASU Experiments”, Blair Johnson
Do you have any questions?

Eglin Blast Pad simulation by CMT-nek
CMT-nek Development and Application

Jason Hackl
David Zwick

CMT-nek development team

Prof. Paul Fischer, UIUC
Jason Hackl, UF
David Zwick, UF
Li Lu, UIUC
Brad Durant, UF
Goran Marjanovic, UF
Rahul Koneru, UF

Postdoctoral fellow Nguyen Tri Nguyen arrives December 10th, 2017
Outline

- CMT-nek hydrodynamics
  - Discontinuous Galerkin spectral element method
  - Euler equations + entropy viscosity method (EVM)
- Microscale release
  - Shock waves and interactions of waves with spheres
- CMT-nek particles
  - Multiphase source terms
  - Algorithms and parallelization
- Mesoscale release
  - ASU experiment

Discontinuous Galerkin SEM

1. Inner product with test function \( v \)
2. Integrate by parts on hexahedral \( \Omega_e \)
3. Numerical flux \( \mathbf{H}^* \) in surface integral
   - Weak boundary conditions
   - Couples elements together
4. Isoparametrically map \( \Omega_e \) to \([-1,1]^d\)
5. Approximate integrals with quadrature
6. Approximate \( U \) & \( v \) with Lagrange polynomials
   - \( N \) Gauss-Legendre-Lobatto (GLL) nodes
   - Nested tensor product \( \sim O(N^d) \)

\[ \frac{\partial U_i}{\partial t} + \nabla \cdot \mathbf{H}_i (U, \nabla U) = R_i \]

\[ \mathbf{H}_i = \mathbf{H}_i^e (U) + \mathbf{H}_i^d (U, \nabla U) \]

Matrix ops within \( \Omega_e \)

\[ \int_{\Omega_e} f(x) \, dV = \int_{-1}^{1} f(r) J \, d^3 r \approx \sum_{j=1}^{N} \omega_j f(r_j) \]

\[ \int_{-1}^{1} \frac{\partial U}{\partial t} J \, d^3 r = \int_{-1}^{1} \frac{\partial r_k}{\partial x_j} \frac{\partial v}{\partial r_k} H_j \, d^3 r - \sum_{j=1}^{6} \int_{-1}^{1} \mathbf{H}^* \mathbf{n}_j J A d^2 r + \int_{-1}^{1} v J R J d^3 r \]

### Convective terms in DGSEM

\[
\int_{-1}^{1} v \frac{\partial U}{\partial t} J \, d^3r = \int_{-1}^{1} \frac{\partial v}{\partial x_j} \frac{\partial v}{\partial x_k} H_j J \, d^3r - \sum_{f=1}^{6} \int_{-1}^{1} \nu H^* \cdot n_f J A \, d^3r + \int_{-1}^{1} v R J \, d^3r
\]

\[
v^\top B \left[ \frac{\partial U}{\partial t} \right] = v^\top D^f \{ \nu \} B \left[ r_{k,x,1} \right] \left| H_0 \right| - v^\top E^f B_A \left[ H_1 \nu_i \right] + v^\top B R
\]

- **E**: Restriction op
- **D**: Differentiation op
- **B**: Mass matrix

### Volume fractions of gas and particles

\[
\phi_g = 1 - \phi_p
\]

\[
\lim_{\nu \to 0} \frac{V_p}{V}
\]

...and particles

\[
U = \phi g \left[ \begin{array}{c} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{array} \right]
\]

### Conserved variables to primitive variables

\[
\frac{\phi_g \rho \nu}{\phi_p} = \frac{U_3}{U_1} \text{ to fluxes in the Euler equations of gas dyn.}
\]

### Thermodynamic state

<table>
<thead>
<tr>
<th>Mass</th>
<th>Temperature</th>
<th>Pressure</th>
<th>Total energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_1 = (U_2, U_3, U_4)^T )</td>
<td>( p(\rho, T) )</td>
<td>( \rho )</td>
<td>( E = \int c_v T , dT + \frac{1}{2} u_i u_i )</td>
</tr>
</tbody>
</table>

### Artificial viscosity

Flux = convective + diffusive

\[
H_i = H_i^c(U) + H_i^d(U, \nabla U)
\]

Artificial stress tensor\(^1\) (NOT Navier-Stokes) with AV that tracks the entropy residual

\[
\text{NOT weighted by volume fraction } \phi_g
\]

**Diffusive flux of...**

- **Mass**

\[
H_1^d = -\kappa_\rho \nabla \rho
\]

- **Momentum**

\[
H_{i+1,j}^d = -\left( \rho \nu_s \sigma_{ij} + \kappa_\rho u_j \frac{\partial \rho}{\partial x_i} \right)
\]

\[
\sigma_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}
\]

- **Energy**

\[
H_5^d = -\left( \rho \nu_s \mathbf{u} \cdot \mathbf{u} + \kappa_\rho \right)
\]

\[
\left( \nabla (\rho e) + \frac{1}{2} |\mathbf{u}|^2 \right)
\]

### Due to entropy viscosity

\[
\nu_s = c_E h^2 \frac{|s - \langle s \rangle|_{\infty}}{\Omega_s}
\]

\[
\nu_{max} = c_{max} h \max_{\Omega_s} (|u| + c)
\]

\[
\nu_s = S(\min(\nu_s, \nu_{max}))
\]

\[
\kappa_s = \rho \nu_s
\]

\[
R_s \equiv \partial s / \partial t + \nabla \cdot (u \ s)
\]

\( R_s \) approx by finite diff between RK3 stages'

\[
S(R) = \frac{1}{12} (6R_{r,1,k} + R_{r+1,j,k} + R_{r-1,j,k} + \ldots)
\]

\( \nu_s \) approx by finite diff between RK3 stages'

\[
s = \rho c_v \log (\rho \rho \gamma)
\]

\( C^0 \) by average \( R_s \) at face points. Smooth via

\[
\frac{1}{12} (6R_{r,1,k} + R_{r+1,j,k} + R_{r-1,j,k} + \ldots)
\]

\( \nu_s \) approx by finite diff between RK3 stages'

\[
S(R) = \frac{1}{12} (6R_{r,1,k} + R_{r+1,j,k} + R_{r-1,j,k} + \ldots)
\]

---

\( ^1 \) Guermond & Popov (2014) "Viscous regularization of Euler eqn and entropy principles" J. Appl. Math. 74:284-305

**Diffusive terms in DGSEM**

Quasi-linear flux Jacobian $A$

**Primal form**

**NOT** weighted by volume fraction $\phi_g$

$\Gamma = \bigcup_{\Omega_e}$

Jump $\{u\} = u_\Gamma^+ - u_\Gamma^-$

average $\bar{\{u\}} = \frac{1}{2} \left( u_\Gamma^- + u_\Gamma^+ \right)$


Weighted resid, int by parts $\rightarrow$ primal form $\rightarrow$ DGSEM ops

$$\int_{\Omega_e} v \nabla \cdot \mathbf{H}^d dV \rightarrow I_{KV} - I_{GU} + I_{G^*U}$$

$I_{KV} = \int_{\Gamma} \{\alpha \Gamma v\} \cdot \{\mathbf{v}\} d\Gamma \rightarrow \mathbf{v}^T \mathbf{B}_A \left[ (\mathbf{H}^d \cdot \mathbf{n}) - \{\{\mathbf{H}^d \cdot \mathbf{n}\} \} \right]$  

$I_{GU} = \int_{\Gamma} \{\alpha \Gamma v\} \cdot \{\mathbf{U}\} d\Gamma \rightarrow \mathbf{v}^T \mathbf{D}_J^d \alpha \Gamma v \mathbf{B}_A \left[ \mathbf{U} - \{\{\mathbf{U}\} \} \right] \bar{n}_i$  

$I_{G^*U} = \int_{\Omega_e} \left( \nabla v \right) \cdot \mathbf{H}^d dV \rightarrow \mathbf{v}^T \mathbf{D}_K^d \mathbf{B} \left[ \mathbf{r}_k, x, \mathbf{H}^d \right]$  


**CMT-nek: final form of DGSEM**

Equate coefficients of $\mathbf{v}^T$

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{B}^{-1} \left[ \mathbf{I}^T \mathbf{D}_{M,k}^T \mathbf{B}_M \left[ \mathbf{r}_k, x, \mathbf{n}_i \right] \mathbf{H}_e^c \left( \mathbf{I} \mathbf{U} \right) \right] + I_{KV} + \mathbf{R}$$

$$- \mathbf{B}^{-1} \left[ \mathbf{E}^T \mathbf{T}_{A}^T \mathbf{B}_{M,A} \left[ \mathbf{H}_c^* \left( \mathbf{I} \mathbf{E} \mathbf{U} \right) \right] \mathbf{I}_A \bar{n}_i + I_{GU} - I_{G^*U} \right]$$

Volume: $O(N_{elem} M^4)$  

Surface: $O(N_{elem} M^2)$

Right-hand-side for fully explicit$^1$ TVDRK3 = Surface ops + Volume ops

Restrictive time step due to diffusion number

$$D = \frac{\kappa \Delta t}{h^2}, \quad \min(D, \text{CFL}) < 1$$

Mass matrix is diagonal; all other matrices are element block-diagonal

- Locality, scaling
- Diagonal mass matrix means LHS is **not** exactly integrated (“variational crime”)
- Dealiased convective terms via interpolator $I$ to $M=3(N-1)/2$ Gauss-Legendre nodes$^2$
- Tensor-nesting saves $M^2$ factor in cost of volume operations

---


Shock capturing in CMT-nek

Calibrated $P$, $c_E$, $c_{\text{max}}$ in Sod\(^1\) shock tube

- $\nu$ reaches $\nu_{\text{max}}$ at shock wave
- Less oscillatory than other HODG\(^3\)

Shu-Osher\(^2\) 1D shock-turbulence surrogate

<table>
<thead>
<tr>
<th>$h$</th>
<th>$N$</th>
<th>$t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>9</td>
<td>0.02</td>
</tr>
</tbody>
</table>

CMT-nek convergence and validation

Homentropic vortex: exponential convergence in smooth flow

Two-shock collision, $t = 0.035$: $O(1)$ Empirical order of convergence in $h$ & $p$

<table>
<thead>
<tr>
<th>$h$</th>
<th>$N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>9</td>
</tr>
</tbody>
</table>

Center for Compressible Multiphase Turbulence
**Microscale: Potential flow over spheres**

Tests generalized Faxen theorem\(^1\)

- FCC 10% Volume fraction
- FCC 15% Volume fraction


**Microscale: Mach 3 shock-sphere**

- 220 - element mesh from GridPro, far-field \(h=0.1075d_p\)
- \(N = 5, 125M\) DOF in surrounding 10\(d_p\) x 10\(d_p\) x 10\(d_p\) box
- 8192 cores on Vulcan

<table>
<thead>
<tr>
<th>(C_E)</th>
<th>(c_{\text{max}})</th>
<th>(P)</th>
<th>(\Delta t)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCMT</td>
<td>40</td>
<td>0.5</td>
<td>0.75</td>
</tr>
</tbody>
</table>
**Microscale: Mach 3 shock-sphere**

Temperature contours; color plots of pressure, artificial kinematic viscosity

**CMT-nek transition plan**

- ASU expansion fan (David)
  - Without 4-way coupling (underway)
  - 4-way coupled (CMT-nek runs with PIEP, collision)
- Sandia shock tube (Rahul)
  - Test shock-particle interaction at mesoscale
- Eglin micro/meso (Josh, Brandon)
  - Real-gas EOS
  - Reactive burn
  - Problem setup
- Demonstration problem (Josh, Rahul, Fred)
Transition to CMT-nek – Timeline

<table>
<thead>
<tr>
<th>Task</th>
<th>Year 4</th>
<th>Year 5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NOV</td>
<td>DEC</td>
</tr>
<tr>
<td>Training with CMT-nek</td>
<td>W</td>
<td></td>
</tr>
<tr>
<td>Blastpad Simulation 3D (Hero Run)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Mesoscale Experiment (2D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Mesoscale Experiment (3D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Microscale Experiment (2D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eglin Microscale Experiment (3D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sandia Shock Tube Experiment</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ASU Expansion Fan</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

W Workshop: "A Boot Camp on CMT-nek"

Transition to CMT-nek – CCMT Workshop

A Boot Camp on CMT-nek
November 29, 2017
Organizers: Bertrand Rollin, Jason Hackl

Agenda

- **CMT-nek: Anatomy of the Beast**
  Speaker: Jason Hackl | 12:00 pm – 1:30 pm

- **Lagrangian Particles in CMT-nek**
  Speaker: David Zwick | 1:30 pm – 2:30 pm

- **Running CMT-nek**
  Speakers: Goran Marjanovic and Brad Durant | 2:30 pm – 3:15 pm

- **Post-Processing and visualization in CMT-nek**
  Speakers: David Zwick and Brad Durant | 3:15 pm – 4:00 pm

- **Lesson Learnt from CCMT’s Simulations**
  Speakers: Fred Ouellet and Yash Mehta | 4:00 pm – 5:00 pm

Attendee list

- Paul Crittenden
- Brad Durant
- Giselle Fernandez
- Joshua Garno
- Jason Hackl
- Rahul Koneru
- Yash Mehta
- Goran Marjanovic
- Chandler Moore
- Fred Ouellet
- Brandon Osborne
- Bertrand Rollin
- Prashanth Sridharan
- David Zwick
Multiphase Flow in CMT-nek

- CMT-nek is built on single-phase nek5000
- While not fully resolved, Eulerian-Lagrangian method can simulate a realistic (~$10^9$) particles
- Difficulties related to particle-fluid coupling
  - Physics
  - Numerics
  - Computer Science
- Outline
  - Particle implementation in CMT-nek/nek5000
  - ASU experiment application

Multiphase Source Terms

$$ R = \begin{bmatrix} 0 & f_{pg} \\ \sigma_g : \nabla (\phi_p v) + g_{pg} + q_{pg} \end{bmatrix} $$

Reference Frames

Lagrangian to Eulerian Transfer

Particle-fluid force coupling and energy contribution

Particle-fluid energy coupling

Eulerian particle velocity
**Dispersed Phase**

- For a single particle:

  **Position:**
  \[
  \frac{dX}{dt} = V
  \]

  **Momentum:**
  \[
  M_p \frac{dV}{dt} = \mathbf{F}_{pg} + \mathbf{F}_{un} + \mathbf{F}_c + \mathbf{F}_b
  \]

  **Energy:**
  \[
  M_p C_{p,p} \frac{dT_p}{dt} = Q_h
  \]

**Interpolation**

- Fluid properties need to be evaluated at particle location
- Quasi-steady force:
  \[
  \mathbf{F}_{qs} = \frac{1}{2} \rho_f (\mathbf{u} - \mathbf{V})^2 A_p C_D
  \]

- Interpolation choices:

<table>
<thead>
<tr>
<th>Method</th>
<th>Accuracy</th>
<th>Scalability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>$O(1/N^2)$</td>
<td>$O(1) - O(N)$</td>
</tr>
<tr>
<td>Cubic</td>
<td>$O(1/N^4)$</td>
<td>$O(N) - O(N^2)$</td>
</tr>
<tr>
<td>Lagrange</td>
<td>$O(1/N^{n+1})$</td>
<td>$O(N^n)$</td>
</tr>
<tr>
<td>Barycentric Lagrange</td>
<td>$O(1/N^{n+1})$</td>
<td>$O(N^n)$</td>
</tr>
</tbody>
</table>
Projection

- Process of spreading Lagrangian quantities to the Eulerian reference frame
- Arises from volume filtering used to get multiphase governing equations
- Here, a Gaussian filter is used

\[ a(x) = A(X)g_M(|x - X|) \]

<table>
<thead>
<tr>
<th>A (Lagrangian)</th>
<th>a (Eulerian)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-F_{pg}</td>
<td>f_{pg}</td>
</tr>
<tr>
<td>-G_{pg}</td>
<td>g_{pg}</td>
</tr>
<tr>
<td>-Q_{pg}</td>
<td>q_{pg}</td>
</tr>
<tr>
<td>V_p</td>
<td>\Phi_p</td>
</tr>
<tr>
<td>V_p V</td>
<td>\Phi_p V</td>
</tr>
</tbody>
</table>

Ghost Particles

Idea:
- If a particle is near a MPI rank edge, it will create a copy of itself called a ghost particle
- Sending perspective rather than receiving perspective

(Ghost particles shown in orange boxes)
Algorithmic Scaling

Ideal Setup:
- Uniform flow in a periodic box
- Particle time scale is 10 time steps
- One particle per grid point
- \( N = 5 \) grid points in each direction
- Vulcan (LLNL)
- CS Team will show load-imbalanced cases

Strong Scaling:
- 13 million grid points
- 13 million particles

Weak Scaling:
- 6,250 grid points/rank
- 6,250 particles/rank

Time is averaged over MPI ranks and time steps

---

Algorithmic Scaling

- Strong scaling diverges from ideal due to:
  - 1 element/rank
  - Ghost particles
- Weak scaling diverges from ideal due to:
  - Inter-processor communication from sending particles

Example Profiling
(10,000 rank case from strong scaling)
Particles in Expansion Waves

- Simulation of vertical shock tube with particle bed at bottom
- When diaphragm bursts, particle bed will swell upwards
- ASU team will provide more detail
- Main goals:
  1. Uncertainty study
  2. Physics
  3. High resolution

Prediction (Validation) Metrics

Shock tube (no particles)  Shock tube with particles

Prediction metrics:
- Bed height
- Fluid pressure
Detailed Simulation

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Experiments</th>
<th>Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_0 [m]$</td>
<td>0.64</td>
<td>5.76</td>
</tr>
<tr>
<td>$L_1 [m]$</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>$D_{in} [m]$</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>$h_0 [m]$</td>
<td>-0.3</td>
<td>-0.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Particles</th>
<th>Experiments</th>
<th>Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_p [um]$</td>
<td>[44,88]</td>
<td>[44,88]</td>
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<tr>
<td>$p_f [kg/m^3]$</td>
<td>2,460</td>
<td>2,460</td>
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<tr>
<td>$N_p$</td>
<td>5,033,861,327</td>
<td>229,500</td>
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<table>
<thead>
<tr>
<th>Initial Conditions</th>
<th>Experiments</th>
<th>Simulations</th>
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<tbody>
<tr>
<td>$p_1 [kPa]$</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>$T_1 [K]$</td>
<td>294</td>
<td>294</td>
</tr>
<tr>
<td>$p_3 [kPa]$</td>
<td>101</td>
<td>101</td>
</tr>
<tr>
<td>$T_3 [K]$</td>
<td>294</td>
<td>294</td>
</tr>
<tr>
<td>$\phi_f$</td>
<td>40%</td>
<td>40%</td>
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<table>
<thead>
<tr>
<th>Grid</th>
<th>Simulations</th>
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<tbody>
<tr>
<td>$N_e$</td>
<td>20,000</td>
</tr>
<tr>
<td>$N_{ex}$</td>
<td>800</td>
</tr>
<tr>
<td>$N_{ex}$/N_{ex}$</td>
<td>5</td>
</tr>
<tr>
<td>$N$</td>
<td>6</td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>0.0013</td>
</tr>
<tr>
<td>$\delta f/\Delta x$</td>
<td>2.5</td>
</tr>
<tr>
<td>$\delta f/D_f$</td>
<td>[38,76]</td>
</tr>
<tr>
<td>Ranks</td>
<td>8,192</td>
</tr>
</tbody>
</table>

Initial Results

- Initial Bed Height $(x = -30 \, \text{cm})$
- Experimental Tube Joint $(x = -32 \, \text{cm})$
Planar Averaged Profiles

Observations:

- Reflected/transmitted expansion wave when incident expansion wave head hits bed
- Pressure ahead of bed is nearly constant but lower than standard shock tube
- Possible clustering of particles

Bed Height

Planar Averaging

Threshold

Box Filter
Fluid Pressure Traces

- At the four joints (excluding diaphragm) along the tubes in the experiment we have pressure sensors

Future Work

- Uncertainty quantification
  - Sensitivity of force models, collision models, diameter distributions
- Physics
  - Effect of bed height, pressure ratio, diameter ranges
- High resolution
  - From results a small number of high resolutions simulations will be run
- Numerics
  - Quadrature effects on small-scale resolution
  - Implicit time marching and artificial viscosity
  - Particle initial conditions
Do you have any questions?

High Resolution Simulation

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Experiments</th>
<th>Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_x$ [m]</td>
<td>0.64</td>
<td>5.76</td>
</tr>
<tr>
<td>$L_y$ [m]</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>$D_h$ [m]</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>$h_0$ [m]</td>
<td>-0.3</td>
<td>-0.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Particles</th>
<th>Experiments</th>
<th>Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_0$ [µm]</td>
<td>[44.88]</td>
<td>[44.88]</td>
</tr>
<tr>
<td>$\rho_0$ [kg/m³]</td>
<td>2,460</td>
<td>2,460</td>
</tr>
<tr>
<td>$N_p$</td>
<td>5,033,861,327</td>
<td>73,440,000</td>
</tr>
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<table>
<thead>
<tr>
<th>Initial Conditions</th>
<th>Experiments</th>
<th>Simulations</th>
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<tbody>
<tr>
<td>$P_i$ [kPa]</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>$T_i$ [K]</td>
<td>294</td>
<td>294</td>
</tr>
<tr>
<td>$P_0$ [kPa]</td>
<td>101</td>
<td>101</td>
</tr>
<tr>
<td>$T_0$ [K]</td>
<td>294</td>
<td>294</td>
</tr>
<tr>
<td>$\phi_f$</td>
<td>40%</td>
<td>40%</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Grid</th>
<th>Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_e$</td>
<td>1,280,000</td>
</tr>
<tr>
<td>$N_{ax}$</td>
<td>3,200</td>
</tr>
<tr>
<td>$N_{xy}, N_{xz}$</td>
<td>20</td>
</tr>
<tr>
<td>$N$</td>
<td>6</td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>0.0003</td>
</tr>
<tr>
<td>Ranks</td>
<td>131,072</td>
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</table>
### Uncertainty Quantification

- **Full factorial design**

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Force Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$F_{un} + F_{qs}$</td>
</tr>
<tr>
<td>2</td>
<td>$F_{un} + F_{qs} + F_{am}$</td>
</tr>
<tr>
<td>3</td>
<td>$F_{PIEP}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Collision Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Off</td>
</tr>
<tr>
<td>2</td>
<td>Walls Only</td>
</tr>
<tr>
<td>3</td>
<td>Particles Only</td>
</tr>
<tr>
<td>4</td>
<td>Walls &amp; Particles</td>
</tr>
</tbody>
</table>

- **Configuration Collision Model**
  - Soft-sphere collision model
  - 72 total simulations (3 repeats)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Diameter Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Monodisperse</td>
</tr>
<tr>
<td>2</td>
<td>Polydisperse</td>
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</tbody>
</table>

### Physics Simulations

- **Full factorial design**

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Bed Height</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-30 cm</td>
</tr>
<tr>
<td>2</td>
<td>-20 cm</td>
</tr>
<tr>
<td>3</td>
<td>-10 cm</td>
</tr>
<tr>
<td>4</td>
<td>0 cm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Pressure Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Diameter Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[44,88] $\mu$m</td>
</tr>
<tr>
<td>2</td>
<td>[89,149] $\mu$m</td>
</tr>
</tbody>
</table>

- Parameters chosen to compare to experiments:
  - ASU
  - Literature (Chojnicki et al., 2006)
- 96 total simulations (3 repeats)
Experimental Studies of Gas-Particle Mixtures Under Sudden Expansion

Blair Johnson, Ph.D., Heather Zunino
Ronald Adrian, Ph.D., Amanda Clarke, Ph.D.
Arizona State University

Outline

- Research Objectives
- Experimental Setup & Measurement Techniques
  - Installation of new pressure sensors
  - Synchronization to optical measurements
  - High speed video of particle bed evolution
  - Particle image velocimetry (PIV) of gas
- Results
  - Pressure analysis
  - Particle bed motion
  - Gas velocity
- Summary & Upcoming Work
Research Objectives

- Provide data for validation of numerical simulations developed by CCMT.
- Measure shock wave, expansion wave, incipient particle bed motion and gas flow, and particle motion in $0 < z < D$ (near field), $0 < z < 7D$ (far field), and $z < 0$ (within bed).
- Coordinate with UQ, UB teams to quantify experimental error and gain insight for potential improvements to experimental facility.

Experimental Plan

<table>
<thead>
<tr>
<th>Particle size (μm)</th>
<th>Pressure Ratio $P_4/P_1$</th>
<th>Bed Height (cm)</th>
<th>Measurement Type</th>
<th># of tests</th>
</tr>
</thead>
<tbody>
<tr>
<td>44 – 90</td>
<td>20</td>
<td>37.9</td>
<td>FV</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>32+</td>
<td>EXP</td>
<td>∞</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10.0</td>
<td>PIV</td>
<td>∞</td>
</tr>
<tr>
<td></td>
<td></td>
<td>15</td>
<td>FV</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10</td>
<td>FV</td>
<td>2</td>
</tr>
<tr>
<td>90 – 150</td>
<td>20</td>
<td>37.9</td>
<td>FV</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>32+</td>
<td>EXP</td>
<td>∞</td>
</tr>
<tr>
<td></td>
<td></td>
<td>15</td>
<td>FV</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10</td>
<td>FV</td>
<td>2</td>
</tr>
<tr>
<td>150+</td>
<td>20</td>
<td>10.0</td>
<td>PIV</td>
<td>∞</td>
</tr>
</tbody>
</table>

FV = Front Rise Velocity
EXP = Bed Expansion Video of Crack/Void Evolution
PIV = Particle Image Velocimetry for gas velocity
Experimental Setup

Vacuum Chamber

Low pressure ($P_1$) above diaphragm

~ 130 cm

Polypropylene Diaphragm

$P_4 = P_{\text{atm}}$ below diaphragm

Glass Spheres $D_{50} = 44\mu m$ to $300\mu m$

4 cm

Apply current to remove diaphragm

Center for Compressible Multiphase Turbulence
**Experimental Setup**

- **Vacuum Chamber**
  - *Vacuum Chamber*
  - *Low pressure (P₄) below diaphragm*
  - *4 cm*

- **Pressure Sensors**
  - *Pressure Sensors (200 kHz)*
  - *~130 cm*

- **Glass Spheres**
  - *D₅₀ = 44μm to 300 μm*

- **Phantom v641**
  - *4-megapixel high speed camera (Fₛ = 10,000+ fps)*

---

**Experimental Setup**

- **Vacuum Chamber**
  - *Vacuum Chamber*
  - *Low pressure (P₄) above diaphragm*
  - *4 cm*

- **Pressure Sensors**
  - *Pressure Sensors (200 kHz)*
  - *Phantom v641* (4-megapixel high speed camera)
  - *Fₛ = 10,000+ fps*
Experimental Setup

Vacuum Chamber

Pressure Sensors (200 kHz)

Phantom v641
4-megapixel high speed camera
($F_s = 10,000+ \text{ fps}$)

Expansion of particle bed

Escape/ris e of interstitial gas

Shock

Rarefaction Wave

Center for Compressible Multiphase Turbulence
Measurement Techniques

- Pressure sensors
- High-speed (10 kfps) video
  - Particle bed expansion
  - Front velocity
- Particle image velocimetry (PIV) of gas in expansion region at top of particle bed

Dynamic Pressure Sensors

- Static pressure sensor
  Omega DPG9145-15
  Pressure above diaphragm (below ~ atmospheric)
- Holes built into diaphragm joint ensure $P_4 = P_{atm}$
Dynamic Pressure Sensors

- Static pressure sensor
  Omega DPG9145-15
  pressure above diaphragm
  (below ~ atmospheric)
- Dynamic sensors
  PCB113B28, Fs = 200 kHz
- Use shock to trigger/sync
  optical measurements
- Detect lateral variations of
  shock and expansion
  waves (UQ, simulation)
Pressure Sensors / Synchronization

- 8 pressure sensors (PCB 113B28) read simultaneously into LabView via PXIe-4492
- Pressure threshold set in LabView (UQ, simulation)
  - Shock trigger for particle bed measurements
  - Expansion trigger for gas PIV

- Hardware trigger sent from PXIe-4492 to PXIe-6341, to BNC-2120, to BNC 565 pulse/delay generator, and to Phantom v641 camera
- Trigger received by camera to initiate optical recording
High speed video

Left: Bed rise

Right: Void development

$F_s = 10,000$ fps

Particle Image Velocimetry (PIV)

Image 1  $\Delta t = 80$ $\mu$s  Image 2
Particle Image Velocimetry (PIV)

- Gas velocity above particle bed, within interstices in top layers of particle bed
- 10 μm silver-coated hollow glass spheres
- Seeded at top of bed, injected above bed

Vacuum Chamber

Double-pulsed Nd:YAG laser

Pressure Sensors (200 kHz)

10 cm

32 cm
Particle Image Velocimetry (PIV)

- Gas velocity above particle bed, within interstices in top layers of particle bed
- 10 μm silver-coated hollow glass spheres
- Seeded at top of bed, injected above bed
- Triggered in expansion
- Synchronization via BNC 565 pulse/delay generator

Field of view: 4 cm x 4 cm, above 10cm bed
Δt ~ 80 μs
F_s = 14 Hz (limited by laser)
Particle Image Velocimetry (PIV)

- Field of view: 4 cm x 4 cm, above 10cm bed
- $\Delta t \approx 80 \mu s$
- $F_s = 14$ Hz (limited by laser)

- $F_s = 14$ Hz $\rightarrow$ Adjust time delay between expansion wave trigger and initiation of PIV
- Explore repeatability based on delay time (UQ)
- Build spatio-temporal record of velocity fields
Outline

- Research Objectives
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  - Pressure analysis
  - Particle bed motion
  - Gas velocity
- Summary & Upcoming Work

Results – Pressure Sensors

[Graphs and images showing pressure sensor data over time]
Results – Pressure Sensors

Results – Wave Speeds

$V_{\text{shock}} \sim 500 \text{ m/s}$

$V_{\text{exp}} \sim 12 \text{ m/s}$ (through particle bed)
Results – Flatness of Shock

Results – Pressure Sensors
Results – Pressure Sensors

Results – Particle Bed Front Velocity

- \( P_2/P_1 = 20; P_1 \approx 5 \text{ kPa} \)
- Track bed height as a function of time,
  \( \sim 60\% \) intensity
- Cubic fit to experimental data
**Results – Particle Bed Front Velocity**

- $P_d/P_1 = 20; P_1 \sim 5 \text{ kPa}$
- 8 experiments of identical conditions

**Results – Particle Bed Packing**

- Able to measure mass/volume in laboratory, but not packing density, porosity, etc.
- Volume fraction of particles
- Segregation of particles by size
Results – Particle Bed Packing

- Threshold method suggests ~59% packing density
- Previously estimated 61%

- Identifies location and radius of each particle
- Volume fraction ~53%
Results – Particle Bed Packing

- Faster bed rise near edges of shock tube
- Faster escape of “cloud” particles in gas velocity near edges
- Lower packing density near walls could explain faster air flow, both gas/particle velocities
Results - Gas Velocity

Outline

- Research Objectives
- Experimental Setup & Measurement Techniques
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  - Synchronization to optical measurements
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- Results
  - Pressure analysis
  - Particle bed motion
  - Gas velocity
- Summary & Upcoming Work
Summary & Upcoming Work

- Synchronization between pressure sensors (via shock or expansion waves) successful with optical measurements (high-speed video, PIV)
- Bed motion can be observed prior to shock wave
- Shock wave self-corrects and shows no lateral variation at pressure sensors 32 cm above diaphragm
- Still pursuing bed packing structure near walls; impact on particle & gas velocity differences at walls
- Possible future experimental update: replace one glass segment with acrylic tube to measure evolution of expansion wave speed

ASU Experimental Team

Heather Zunino
Blair Johnson
Ron Adrian
Amanda Clarke
Do you have any questions?
AFRL/RW Experiments

Angela Diggs

Outline

• FY17 Macroscale Experiment
  • Test Set-up & Instrumentation
  • Results & Analysis
    • High Speed Video
    • Pressure Transducers
  • Future Work
• FY18 Microscale Experiment
  • Test Set-up
  • Instrumentation
**Motivation**

- **Frost [1]**
  - Instrumentation
    - High speed cameras
    - Far field pressure probes
  - Detonation
    - Charge mass = 2.4g
    - Glass mass = 240g
      - M/C = 100
    - Steel mass = 10.5kg
      - M/C = 4400

- **Desired**
  - Instrumentation
    - High fidelity data for model development and validation
    - Large quantity of data collected at near field
  - Proposed solution
    - AFRL/RW Blast Pad: pressure probes, high speed cameras, additional instrumentation for momentum
    - Match legacy Comp B charges for cost savings
      - Charge mass = 8.55lb

**Outline**

- FY17 Macroscale Experiment
  - Test Plan & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
  - Future Work
- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation
AFRL Blastpad Experimental Setup

- Instrumentation:
  - Pressures probes
  - Momentum traps
  - Four high speed video cameras
  - Linear optical transducers

- Six shots
  - 2 bare charges
  - 1 charge w/tungsten (notched)
  - 1 charge w/steel (un-notched)
  - 2 charges w/steel (notched)

Blastpad Test Articles

- The ratio of the mass of the particles to the mass of the charge (M/C ratio) is critical to expected behavior
- Literature review (Frost, Zhang) indicates instabilities will be present for M/C ≥ 10
- The charge mass matches legacy blastpad data (released to UF for UQ analysis)

Dimensions in inches

a) bare charge
M = 4.1kg  
b) Charge w/tungsten particles
M/C = 10  
c) Charge w/steel particles, M/C = 13
Test Article Casing

- Case fracture may be a possible mechanism for jetting instability [Zhang et al. 2001, Xu et al. 2013]
- Case influence was minimized by using 3/16” phenolic tubing (notches were 1/32”)

Preliminary Particle Characterization

- **Steel Particles**
  - Multiple vendors surveyed. Criteria were high particle roundness (sphericity) and narrow particle spread
  - Vendor: Osprey Sandvik
  - Size range (confirmed with particle sizer): 75-125 µm
  - SEM shows mostly spherical particles

- **Tungsten Particles**
  - Government provided
  - Size range (confirmed with particle sizer): 100-130 µm
  - SEM shows mostly spherical particles
### Uncertainty Quantification

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explosive length [mm]</td>
<td>AFRL measurement</td>
</tr>
<tr>
<td>Explosive diameter [mm]</td>
<td>AFRL measurement at 5 locations</td>
</tr>
<tr>
<td>Explosive density [kg/m³]</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Explosive quality</td>
<td>AFRL X-ray</td>
</tr>
<tr>
<td>Particle diameter [mm]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle density [kg/m³]</td>
<td>CCMT measurement</td>
</tr>
<tr>
<td>Particle volume fraction</td>
<td>AFRL calculation</td>
</tr>
<tr>
<td>Ambient pressure [kPa]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Ambient temperature [C]</td>
<td>AFRL weather station</td>
</tr>
<tr>
<td>Probe locations [m]</td>
<td>CCMT measurement</td>
</tr>
</tbody>
</table>

Pre-test collaboration ensures input parameter measurements are performed to quality requested by UF CCMT UQ team.

### Outline

- FY17 Macroscale Experiment
  - Test Set-up & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
- Analysis
- Future Work
- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation
Pressure Transducers & Cameras

Cameras 1 & 4
- Phorotron V1212
- 12000 fps

Cameras 2 & 3
- Phorotron V711
- 7500 fps

Bare Charge Video
Tungsten & Steel Liner Videos

- Tungsten Liner
  - Instabilities present
  - Luminosity from particles
- Tungsten Particles
  - Instabilities present

Pressure Transducer Analysis

- Peak pressure (PP) recorded for each pressure transducer (green)
- Shock time of arrival (TOA) when 50% of the maximum pressure is reached (red)
- Manual corrections applied to noisy data

E line pressures (perpendicular) for position 1 (near, left) & 7 (far, right).
Legacy Data

- Comparison performed along the E line (perpendicular)
- Constant shape and weight of Comp B

Legacy data may be used to calculate uncertainties with confidence.

Effect of Notched Casing

- Some variability
- No clear, consistent trends

Case notches do not appear to have an effect. Analysis may assume 3 repeats of steel liner shots.
Shot Comparison

- Data point = average
- Vertical error bars = 1σ
- Steel = 3 repeated shots
- Bare charge = 4 repeated shots

Momentum transfer to particles lowers peak pressure in near field and slows the shock speed.

Outline

- FY17 Macroscale Experiment
  - Test Set-up & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
  - Future Work
- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation
Additional Blastpad Analysis

- High Speed Video
  - Shock front tracking
  - Particle front tracking
  - Analysis of instabilities

- Pressure Transducers
  - Pressure contours
  - Impulse calculations

- Unconfined momentum traps
  - Particle & gas momentum

- Optical linear encoders
  - Particle & gas momentum

Outline

- FY17 Macroscale Experiment
  - Test Set-up & Instrumentation
  - Results & Analysis
    - High Speed Video
    - Pressure Transducers
  - Future Work

- FY18 Microscale Experiment
  - Test Set-up
  - Instrumentation
Future Experiments

- Previous feedback from AST/TST shows concern with modeling the compaction regime
- Future experiments at lower volume fraction will allow a focus on multi-disperse effects, vice compaction
  - 20% volume fraction explosive experiments
  - Motivated by Multiphase Shock Tube at Sandia, but explosively driven
  - Additively manufacture test articles to achieve low volume fraction
  - Microscale experiments due to AFRL budget constraints

Future Experiments

- Instrumentation
  - High Speed Videos
  - Pressure Transducers
  - X-rays
  - Schlieren Imaging
Conclusions

- Blastpad data analysis ongoing
- AFRL/RW approved funding for FY18 microscale experiments
- Close coordination between UF and AFRL/RW ensures relevant experimental data is collected for model development and validation

---

Do you have any questions?
Tungsten Liner Video

Tungsten Liner Video (Backup)
Uncertainty Budget
Validation and Uncertainty Reduction

Chanyoung Park, Raphael (Rafi) T. Haftka and Nam-Ho Kim
Department of Mechanical & Aerospace Engineering,
University of Florida

Integrated Uncertainty Budget Team

- PI: Raphael T. Haftka and Nam-Ho Kim
- Research Scientist: Chanyoung Park
- Graduate students
  - Kyle Hughes (UQ of Eglin exp.)
  - Justin T. Mathew (UQ of ASU/SNL experiments)
  - Samaun Nili (Mesoscale 1D/2D simulations and convergence)
  - Yiming Zhang (Validation and UQ of BE emulation)
  - Giselle Fernandez ( Macroscale sensitivity study)
- Undergraduate student
  - Shirly Spath (UQ of Eglin exp.)
**Sequence of Events and Key Physics Models**

**Detonation phase**
- **T1**: Detonation model
- **T2**: Multiphase turbulence model
- **T4**: Collision model
- **T5**: Compaction model

**Dispersion phase**
- **T3**: Thermodynamics and transport model
- **T6**: Particle force model
- **T7**: Point particle thermal model
- **T8**: Deformation model

**Key physics models**
- Red: Key physics models
- Gray: Other physics models

---

**Planned Sim/Exp Interactions and Progress**

- Model validation for each scale based on UQ, **uncertainty reduction** and **error reduction** through model improvement
- Carrying out Sims/Exps interactions for the key physics models

**Macro scale**
- Eglin Macroscale Simulations
- Eglin Macroscale Experiments

**Mesoscale**
- ASU Vertical Shocktube Experiments
- SNL Mesoscale Simulations
- SNL Shocktube Experiments
- Eglin Mesoscale Simulations
- Eglin Gas gun Experiments

**Microscale**
- Characterize Particle Bed
- Characterize Particle Curtain
- Characterize Particle Bed
- Characterize Particles After Detonation

**Characterization & Calibration**
- In progress

**Plans**
- ???
### Hierarchical Validation and U Propagation

- **VVUU framework**
  - Target model

![Diagram showing hierarchical validation and U Propagation]

### Integrated UQ Accomplishments

- **UQ of experimental measurement processing**
  - Propagating uncertainty when desired measurements are obtained by processing proxy data
  - Planning experiment to better expose uncertainty in measurements
  - Involvement of UQ team in measuring uncertainty in experiments

- **Help verification by enabling convergence**
  - Achieving convergence of the mesoscale multiphase flow simulation by modeling effect of finite size of particles

- **Preparation for UQ of macroscale simulation**
  - Multi-fidelity surrogate
  - Also useful for exascale behavioral emulation
UQ of Measurement Processing

- Desired measurements obtained by processing proxy data
  - **Sandia** shocktube experiment: Volume fraction measuring requires processing from X-ray images
  - **ASU** mesoscale experiment: Reducing uncertainty in diaphragm burst time \((t=0)\) by placing pressure sensors
  - Planning **Eglin** macro experiments for reducing uncertainty in experimental measurements

- **Involvement of UQ team in measurement processing**
  - **Eglin/ASU** experiment: Measuring volume fraction with CT scanner, particle size with SEM images and particle density with pycnometer at UF
Verification of Particle Force Model

- Experiments → Experimental input → Input uncertainty → Simulations
- Target model

- Quantification of numerical error
  - Achieving convergence to obtain discretization error of the Sandia shocktube simulation
  - Modeling finite volume particles

- Sampling uncertainty
- Measurement uncertainty
- Measuring process uncertainty

- Uncertainty/error reduction
- Large?

UQ of Expensive Macroscale Simulation

- Experiments → Experimental input → Input uncertainty → Simulations
- Target model

- UQ using multi-fidelity surrogate
  - Multi-fidelity surrogate provides an approach for simulating expensive simulations cheaply
  - Applying on the UQ-exascale interaction

- Sampling uncertainty
- Measurement uncertainty
- Measuring process uncertainty

- Uncertainty/error reduction
- Large?

- Propagated uncertainty
  - Stochastic variability
  - Discretization error
  - Neglected feature/physics
UQ of Measurement Processing

UQ involvement in experiments
We found that the maximum volume fraction was used with 'top-hat' profile in the Sandia shock tube simulations. Dominant uncertainty in the maximum volume fraction. Bell shaped profiles (little uncertainty in the symmetricity). Reduced the uncertainty in the maximum volume fraction.

Goal: Quantifying and modeling uncertainty in the measuring process of initial volume fraction and profile shape (Justin Mathew).

Volume fraction was calculated based on intensity ratio using the Beer-Lambert law and calibration experiment. $-A \rho d = \ln \frac{I}{I_0}$

$A$: Attenuation coefficient
$\rho$: Particle density
$d$: Distance through particles
$
\phi$: Volume fraction

$\tau$: Curtain thickness

$\tau = \phi t$
Calibration of A for Measuring VF

- A constant attenuation coefficient does not fit the measured data well due to beam hardening

Wagner et. al (2015)

- **Goals:** Estimating the true trend and quantifying the uncertainty in the prediction

\[
A(I/I_0) = \frac{\ln I/I_0}{-\rho d}
\]

Calibrated A for Measuring VF

- Assumed correlated **noise in the data**
- Made prediction of A and its uncertainty using a Gaussian process model
- Considered linear and quadratic polynomial models (model form uncertainty)
- Obtained random attenuation curves based on the correlated noise model with Monte Carlo simulations
Uncertainty in Initial Volume Fraction

- Two models gave similar results: little model form uncertainty
- The uncertainty in the attenuation coefficient was propagated mostly in the uncertainty of the maximum volume fraction
- The uncertainty in the volume fraction profile was modeled with radial basis function networks (RBFN)

Variability in VF

Linear model

RBFN Regression

Implementing the bell shaped profile for simulations

Summary of Sandia Mesoscale Campaign

- Sandia campaign has been almost completed
- Found and reduced 1) the hidden error due to the use of AUSM+ and 2) the uncertainty due to the gaps
- Uncertainty in the initial volume fraction is the currently largest uncertainty source in the model error estimate (down stream position)

Implementing the bell shaped profile for simulations
UQ of Measurement Processing

- Macroscale
- Mesoscale
- Microscale

Characterization & Calibration

- Characterize Particle Bed
- Characterize Particle Curtain
- Characterize Particle Bed
- Characterize Particles After Detonation

Eglin Macroscale Simulations
Eglin Macroscale Experiments
Eglin Macroscale Simulations
Eglin Macroscale Experiments
Eglin Macroscale Simulations
Eglin Macroscale Experiments
Eglin Microscale Simulations
Eglin Microscale Experiments
Eglin Microscale Simulations
Eglin Microscale Experiments

UQ Involvement in ASU Experiment

- Goals:
  - Plan new validation experiments that consider simulation limitations and uncertainty quantification goals (Justin Mathew)
  - Identify sources of experimental uncertainty, quantify those suspected to have a greatest influence on simulation inputs (Justin Mathew, Kyle Hughes)
  - UQ is involved in the experiment

- Shock tube overview:
  - Four 32cm length segments
  - Particle diameter: 45-90 microns
  - Pressure ratio: ~20
  - Initial bed height: 32 cm
Uncertain Experimental Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Quantity</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diaphragm burst time</td>
<td>?</td>
<td>Pressure sensor</td>
</tr>
<tr>
<td>Volume of particle bed</td>
<td>383.5-385.6 cm³</td>
<td>CT scanner</td>
</tr>
<tr>
<td>Initial volume fraction</td>
<td>59-65%</td>
<td></td>
</tr>
<tr>
<td>Initial mean volume fraction</td>
<td>60-61%</td>
<td></td>
</tr>
<tr>
<td>Particle diameter (before)</td>
<td>67±8 μm</td>
<td>SEM</td>
</tr>
<tr>
<td>Particle diameter (after)</td>
<td>68±22 μm</td>
<td>SEM</td>
</tr>
<tr>
<td>Particle density</td>
<td>2.44±0.006 g/cm³</td>
<td>Pycnometer</td>
</tr>
<tr>
<td>Driver section pressure</td>
<td>100.68±? kPa</td>
<td></td>
</tr>
<tr>
<td>Driven section pressure</td>
<td>5.5±? kPa</td>
<td></td>
</tr>
<tr>
<td>Tube geometry</td>
<td>Negligible</td>
<td></td>
</tr>
</tbody>
</table>

- **Justin Mathew** and **Kyle Hughes** actively involved in measuring the uncertainties

Particle Characterization – Shape/Size

- Glass particles: 45-90 microns in diameter, 2.44±0.006 g/cm³ (**Kyle Hughes** and **Justin at UF**)
- Scanning electron microscope (SEM) Images show largely homogenous groups of particles with no apparent source of significant variation (**Kyle**)

Scanning SEM images of particles after the experiment
Particle Bed Characterization – Initial VF

- To verify estimates of ~61% average volume fraction measured during ASU experiments, a mock particle bed was created for a CT scan
  - The mock tube was only 7 mm in diameter (versus ~40 mm shock tube diameter)
  - Observed a mysterious volume fraction increase in the radial direction

Preliminary Comparison and UQ

- There is inconsistency in measuring the bed heights
- The height data from the experiments is based on high speed camera image while the simulation predicts height data based on volume fraction prediction
- The uncertainty in t=0 has to be quantified accurately
New Experiment Planning

- New experiments are conducted considering simulation limitations and UQ goals
  - Usage of smaller particle sizes (45-90 micron) to speed up simulation time
  - Pressure probes distributed to reduce uncertainty in diaphragm burst timing
    - 1-3-2-2 distribution of pressure probes
    - The lesson learned from UQ of the Eglin microscale experiment
  - Additional 2-3 cm of bed height added above the clamp for better optical range

UQ of Measurement Processing
Eglin Microscale Experiments

Schematic top-view of the test set-up.
Source: Black, Littrell, and Delcambre, internal written report, 3/7/2015

- With a small number of particles, surprising evidence that the flow is strongly coupled with particles:
  - Mean shock arrival times increase as the number of particles is increased
- A possible explanation is high volume fraction in the initial plane of the particles:

UF Analysis of Particles Used in Eglin

- Eglin mesoscale gas gun experiment
  - CT scans of particle packet, SEM of particles, particle density via pycnometer
  - Simacon and X-ray images to track particle cloud movements

- Eglin macroscale blastpad experiment
  - SEM of particles and particle density via pycnometer
  - Steel mock CT scan
  - Comp B X-rays

SEM of several steel particles at 500x zoom.
75-125 µm Steel
Controlling Casing Influence

- Casing fracture may be a possible mechanism for jetting instability
- No significant effect from analytical estimation
- Steps taken to reduce the influence of the casing:
  - Thin phenolic tubing (3/16") for the casing
  - Failure energy ~0.06% of explosive energy
  - No casing between the explosive and particles
  - Casing notched on outer surface to control case failure

<table>
<thead>
<tr>
<th>Shot</th>
<th>Liner</th>
<th>Notched?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>Tungsten</td>
<td>Y</td>
</tr>
<tr>
<td>4</td>
<td>Steel</td>
<td>Y</td>
</tr>
<tr>
<td>5</td>
<td>Steel</td>
<td>Y</td>
</tr>
<tr>
<td>6</td>
<td>Steel</td>
<td>N</td>
</tr>
</tbody>
</table>

Quantification of Numerical Error
Achieving convergence by modeling finite size particles
Summary and Overview

- **Goal:** To achieve force convergence in a two-way coupled point particle Euler-Lagrange simulation using the finite size of the particles and to estimate the numerical error in the point-particle force (Samaun Nili)

- In the point particle method, the particle feels the shock only if the shock reaches to the cell where particle center is located.
- When the particle diameter is larger than the grid size, the particle force shows an unrealistic jump at the center.
- The peak force increases as we reduce the grid size.
Proposed Solution

- The inhomogeneous flow felt by the particle represented by average over the surface or volume of the particle (Faxen theorem)
- Computing the average volume and surface gas quantities and forces
- The numerical solution compared against the analytical solution

---

**QS Force with Single Particle (115μm)**

**Point particle**

- $f_q$ vs. time ($t^* = t/(D_p/U_s)$)

**Finite size particle**

- $f_q$ vs. time ($t^* = t/(D_p/U_s)$)
Quasi-Steady Force Convergence

- RMSE measures the difference between analytical solution and finite size point particle model
- RMSE decreases exponentially

![Graph showing RMSE (kN/kg) vs. particle diameter (µm)]

Preparation for UQ of Macroscale Simulation

With Multi-Fidelity Surrogate
Multi-Fidelity Surrogate for UQ

- UQ often computationally expensive since it requires numerous simulation runs
- Surrogates often provide good approximations based on several dozens of samples but even sampling for building a surrogate is not affordable for expensive simulations
- **Multi-fidelity surrogate**: Approximating an expensive high fidelity simulation behavior by combining a few expensive high fidelity samples with cheap low fidelity samples
- **Low fidelity model selection**: There are multiple lower fidelity models and selection is another question to be answered
- This technique is used for the collaboration with the exascale team to approximate the CMT-bone with CMT-bone-BE and BE emulation
Introduction to Multi-Fidelity Surrogate

- **Goal:** Approximating the high fidelity response based on a few high fidelity samples with low fidelity samples

\[ \hat{y}_H(x) = \rho \hat{y}_L(x) + \delta(x) \]

- \( \hat{y}_H(x) \): High fidelity simulation prediction
- \( \hat{y}_L(x) \): Low fidelity simulation prediction
- \( \delta(x) \): Discrepancy prediction

MFS for UQ of 3D Sandia Shocktube Sim.

- **Goal:** Approximating the 3D simulation for predicting front positions using 1D and/or 2D simulations
- The simulations have the same grid resolution

Simulation parameters:
- Volume fraction
- Curtain thickness
- Mach number
- Random initial particle position

- 15 (3D) / 135 (2D) / 625 (1D)
- Computational cost ratios:
  - A single 3D run is equal to 25000 1D runs or 100 2D runs
  - A single 2D run is equal to 250 1D runs
MFS Accuracies with 1D+3D and 2D+3D

- Predicting **downstream front position** at 700 μs
- Using 11 other 3D runs to evaluate accuracy in terms of **relative RMSE** (RMSE/max value)
  - 0.025 (1D+3D) and 0.0875 (1D only)
  - 0.0125 (2D+3D) and 0.0375 (2D only)
  - 0.0638 (3D only)

**DOE:** 1D (125) + 3D (4)

**DOE:** 2D (27) + 3D (4)

**Difference Between 1D/2D/3D**

- MFS prediction allows to **predict difference** between models of different fidelities
- For the shock tube simulation, the difference is most sensitive to Mach number
- The difference between 3D and 1D is higher than that between 3D and 2D
Summary

- Involvement of physics and UQ for experimental data extraction through measurement processing
  - The initial volume fraction of the Sandia shock tube experiment extracted from X-ray images using a X-ray attenuation model
  - Rigorous UQ has reduced the initial uncertainty by 50%

- Involvement of UQ team in measurement processing
  - UQ of the ASU and Eglin experiments
  - Planning those experiments for reducing measurement uncertainty

- Quantifying numerical error in the particle force model by modeling finite size particles

- Carrying out a study on Multi-fidelity surrogate for UQ and parametric study of hero simulations and BE emulation development

---

**Do you have any questions?**
### Computation Cost

- **3D**
  - $dx=dy=dz=125\mu\text{m}$
  - Length x Width x Height = 0.35 0.04 0.01 (M=1.45, 1.24)
  - Length x Width x Height = 0.38 0.04 0.01 (M=1.92)
  - 6 million particles
  - Quartz 2048 cores wall time 24 hrs (max), 23 hrs +/- 20 mins

- **2D**
  - $dx=dy=dz=125\mu\text{m}$
  - Length x Width x Height = 0.35 0.04 125\mu\text{m} (M=1.45, 1.24)
  - Length x Width x Height = 0.38 0.04 125\mu\text{m} (M=1.92)
  - 600,000 particles
  - Vulcan 128 cores wall time 40 hrs

- **1D**
  - $dx=125\mu\text{m}$
  - Length = 0.35 (M=1.45, 1.24)
  - Length = 0.38 (M=1.92)
  - 5000 particles
  - Hipergator 4 cores wall time 20-30 mins

---

### 1D/2D/3D Front Position Comparisons

- Comparing 1D/2D/3D for two extreme combinations in terms of prediction metric (mean front positions)
  - M=1.24, 14%, 1.5 mm and M=192, 18%, 3.5 mm
  - Variability due to initial particle positions is small for 1D and negligible for 2D

![Mean front positions](image)

- **Mean front positions (M=124, 14%, 1.5 mm)**
  - 1D
  - 2D
  - 3D

- **Mean front positions (M=192, 18%, 3.5 mm)**
  - 1D
  - 2D
  - 3D
Slices from CT scan vs Rocpack

Mock Bed - CT  
Rocpack - CT

PVF Calculated Along Circular Region

<table>
<thead>
<tr>
<th>Region</th>
<th>PVF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Red</td>
<td>0.566</td>
</tr>
<tr>
<td>Blue</td>
<td>0.544</td>
</tr>
<tr>
<td>Yellow</td>
<td>0.568</td>
</tr>
<tr>
<td>Green</td>
<td>0.557</td>
</tr>
<tr>
<td>Cyan</td>
<td>0.562</td>
</tr>
<tr>
<td>Magenta</td>
<td>0.540</td>
</tr>
</tbody>
</table>

Nominal PVF = 0.54
CMT-nek: CS Update

Sanjay Ranka
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University of Florida
sanjayranka@gmail.com
352 514 4213

Members

Keke Zhai
Mohamed Gadou
Adeesha Malavi
Tania Banerjee

Aravind Neelakantan
Sai Chenna
Sanjay Ranka
Key Accomplishments (past year)

- Dynamic load balancing of CMT-nek
- Hybrid Multicore Computing using DVFS
- Multi-level Memories and performance impact

Exascale Simulation: CS Challenges

Dynamic Load Balancing

Energy and Performance Tradeoffs

Future Architectures and Hybrid Processors

Parallelization on a million+ processors
Talk Overview

- CMT-bone/CMT-nek
- Dynamic Load Balancing
  - Colocation of particles with spectral elements
  - Mapping/Remapping
- Hybrid Multicore Processor
  - Hybrid Core Mapping
  - KNL (Multi-level Memories)
  - Power/Energy Modeling
  - Dynamic Voltage Scaling
  - Traditional Core (Autotuning)
  - GPU (Manual Tuning)
- Conclusions

CMT-bone

Each cube represents a spectral element – formulation of the finite element method that uses high degree piecewise polynomials as basis functions.

Performance per Watt Improvement

- Dynamic Load Balancing
- Multi-Level Memories
- Power/Energy Performance Trade offs
- Dynamic Voltage Scaling
- CMT-nek CMT-bone
- Hybrid Core Mapping
- Dynamic Load Balancing
- Auto Tuning

Dynamic Load Balancing: Expansion Fan
Hero Run 2

Dynamic Load Balancing

- Initialization
  - Elements to processor mapping
- Repeat the following steps
  - Decide when to trigger a remap
    - Rebalance after every k time steps
    - Rebalance when processing time per step gets higher beyond a threshold
  - If remap trigger = yes
    - Derive new elements to processor mapping
- Transfer elements and particles and reset other data structures
  - Serialize
  - Communication
  - Deserialize
- Final Steps
Serialization using Spectral Bisection

Elements to Processor Mapping

(a) Default elements to processor mapping, agnostic of particles
(b) Elements to processor mapping, after taking into account both elements and particles

The Centralized Algorithm

Initially, each processor has an element load array

Element load = # particles + fluid load
The Centralized Algorithm

Each processor sends element load array to P0

P0 receives and concatenates the element load array, computes the prefix sum, divides prefix sum by average load
**The Centralized Algorithm**

P0 distributes the assignment to other processors, and each processor gets the new elements

P0

3  6  4  5  8

P1

8  10

P2

8  7  3  7  3

---

**The Distributed Algorithm**

Each processor computes local prefix sum and the exclusive prefix sum of the element load on each processor

P0

3  9  13  18

Exclusive prefix sum

18  34  20

Prefix sum

0  18  52

P1

8  16  26  34

P2

7  10  17  20
The Distributed Algorithm

Each processor adds the exclusive prefix sum to local prefix sum array to get the global prefix sum of element load array.

```
<table>
<thead>
<tr>
<th>P0</th>
<th>0</th>
<th>18</th>
<th>52</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3</td>
<td>9</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>9</td>
<td>13</td>
</tr>
</tbody>
</table>
```

```
P1
<table>
<thead>
<tr>
<th>8</th>
<th>16</th>
<th>26</th>
<th>34</th>
</tr>
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<tbody>
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<td></td>
<td></td>
<td></td>
<td>18</td>
</tr>
<tr>
<td>26</td>
<td>34</td>
<td>44</td>
<td>52</td>
</tr>
</tbody>
</table>
```

```
P2
<table>
<thead>
<tr>
<th>7</th>
<th>10</th>
<th>17</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>52</td>
</tr>
<tr>
<td>59</td>
<td>62</td>
<td>69</td>
<td>72</td>
</tr>
</tbody>
</table>
```

Each processor divides the global prefix array with the average load (in this case 24).

```
P0
<table>
<thead>
<tr>
<th>3</th>
<th>9</th>
<th>13</th>
<th>18</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>24</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
```

```
P1
<table>
<thead>
<tr>
<th>26</th>
<th>34</th>
<th>44</th>
<th>52</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>24</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>
```

```
P2
<table>
<thead>
<tr>
<th>59</th>
<th>62</th>
<th>69</th>
<th>72</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>24</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>
```

Processor number
The Distributed Algorithm

Each processor keeps the elements that belong to them, and sends the remaining elements to the target processor.

P0
3 6 4 5

P1
8 8 10

P2
8 7 3 7 3

Dynamic Load Balancing for Compressible Multiphase Turbulence, Keke Zhai, Tania Banerjee, David Zwick, Jason Hackl and Sanjay Ranka, submitted to IPDPS 2018

Rebalancing Time: Total Overhead (Quartz)

- Overhead is about 220 and 121 time steps upon using centralized and distributed algorithms respectively.
- When extrapolated to a million ranks, centralized algorithm will take about 2300 time steps, whereas distributed algorithm will take 1800 time steps.

Max: 73,728 MPI ranks
4 elements / rank
343 particles / element
Grid size: 5x5x5
Rarefaction test
Expansion testcase: CMT-nek on Quartz

- Total time taken by CMT-nek is 4.62 hours
- Total time taken by load balanced code is 33 minutes
- Time per time step: 3.33 s for the original versus 0.4 s for the load balanced code (balancing done every 300 s)
- Adaptive load balancing takes about 31 minutes total and 0.37 seconds per time step

Expansion testcase: Power consumption on Quartz (using Libmsr)

- Power consumption is comparable

Power components:
- Original
- Load Balanced

Center for Compressible Multiphase Turbulence
When extrapolated to a million ranks, centralized algorithm will take 5.68s, whereas distributed algorithm will take 2.66s.

Overhead is approximately 9 time steps with centralized and 7 with distributed when 393,216 cores are used.

The original CMT-nek finished 800 steps in 5 hours.
Total time taken by load balanced code is 4.57 hours.
Time per time step: 21.2 seconds for the original versus 3.3 for the load balanced code.
Expansion testcase: Power consumption on Mira (Using MonEQ)

- Core power and DRAM power reduced by about 5% and 2% respectively, leading to an overall reduction of 3.5% of total power when load balancing is used.
- Energy consumption of the load balanced code is better because of reduced time as well as reduced power consumption.

Hybrid Multicore Architectures

Multi-objective Load decomposition

Theoretical formulation

Minimize

\[ E(n, m, f, g, S) \]

Subject to

\[ T(n, m, f, g, S) \leq T_1 - O(n, m, f, g, S) \]

\[ n \leq N \]
\[ m \leq M \]
\[ f \in F \]
\[ g \in G \]

\[ n \] CPU cores, freq \( f \)

\[ m \] GPU cores, freq \( g \)

\[ \times \]

CPU Experiments

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x ), problem size in terms of number of elements (57)</td>
<td>1024, 1152, 1280, 1408, 1536, 1664, 1792, 1920, 2048, 2176, 2304, 2432, 2560, 2688, 2816, 2944, 3072, 3200, 3328, 3456, 3584, 3712, 3840, 3968, 4096, 4224, 4352, 4480, 4608, 4736, 4864, 4992, 5120, 5248, 5376, 5504, 5632, 5760, 5888, 6016, 6144, 6272, 6400, 6528, 6656, 6784, 6912, 7040, 7168, 7296, 7424, 7552, 7680, 7808, 7936, 8064, 8192</td>
</tr>
<tr>
<td>( f ), frequency in MHz (5)</td>
<td>1200, 1500, 1800, 2100, 2400</td>
</tr>
<tr>
<td>( n ), number of cores (5)</td>
<td>1, 2, 4, 8, 12</td>
</tr>
</tbody>
</table>
CPU Experiments

- Time per time step for processing a problem size of 8192 spectral elements and 256,000 particles
- Experiments show time decreases by increasing CPU counts and frequency

CMT-bone
8,192 elements
256,000 particles
Grid size: 7x7x7

---

CPU Experiments

- CPU communication time for processing 8192 spectral elements and 256,000 particles
- Communication time first decreases and then increases as processors are increased because volume of data communicated per core decreases in the beginning but the total communication volume begins to increase later

CMT-bone
8,192 elements
256,000 particles
Grid size: 7x7x7
Assumptions

- Performance using lower clock frequencies may be derived from that using the highest clock frequency
  \[ T_{\text{CPU}}(n, f, x) = k \times \frac{f_{\text{max}}}{f} \times T_{\text{CPU}}(n, f_{\text{max}}, x) \]
- Power consumption does not depend on problem size
  \[ P_{\text{CPU}}(n, f, x) = P_{\text{CPU}}(n, f) \]
- \( n \) = CPU count, \( f \) = CPU frequency, \( x \) = problem size
- Example: Power lookup table:

<table>
<thead>
<tr>
<th>( f )</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>93.24</td>
<td>97.33</td>
<td>101.32</td>
<td>114.46</td>
<td>127.50</td>
</tr>
<tr>
<td>1500</td>
<td>96.67</td>
<td>100.78</td>
<td>108.32</td>
<td>122.95</td>
<td>136.79</td>
</tr>
<tr>
<td>1800</td>
<td>98.14</td>
<td>102.88</td>
<td>111.53</td>
<td>131.86</td>
<td>148.45</td>
</tr>
<tr>
<td>2100</td>
<td>100.69</td>
<td>106.31</td>
<td>117.11</td>
<td>138.72</td>
<td>160.84</td>
</tr>
<tr>
<td>2400</td>
<td>102.65</td>
<td>108.12</td>
<td>123.94</td>
<td>145.54</td>
<td>167.08</td>
</tr>
</tbody>
</table>

Prediction Error

- Prediction error is within 3% for 99% of the tests
- Prediction error is within 5% for 99% of the tests
GPU Experiments

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y$, problem size</td>
<td>Same problem sizes as described for CPUs.</td>
</tr>
<tr>
<td>size in terms of</td>
<td></td>
</tr>
<tr>
<td>number of elements</td>
<td></td>
</tr>
<tr>
<td>($57$)</td>
<td></td>
</tr>
<tr>
<td>$g$, frequency in MHz</td>
<td>875, 810, 745</td>
</tr>
<tr>
<td>($3$)</td>
<td></td>
</tr>
<tr>
<td>$m$, number of GPUs</td>
<td>1, 2, 4, 8</td>
</tr>
<tr>
<td>($4$)</td>
<td></td>
</tr>
</tbody>
</table>

Time per time step for processing a problem size of 8192 spectral elements and 256,000 particles

Experiments show time decreases by increasing CPU counts and frequency
GPU Experiments

- Total communication time when GPUs are used to solve the problem

Assumptions

- Performance using lower clock frequencies may be derived from that using the highest clock frequency
  \[ T_{\text{GPU}}(m, g, y) = k \times \frac{\text{given}}{g} \times T_{\text{GPU}}(m, g_{\text{max}}, y) \]
- Power consumption does not depend on problem size
  \[ P_{\text{GPU}}(m, g, y) = P_{\text{GPU}}(m, g) \]
- \( m = \) GPU count, \( g = \) GPU frequency, \( y = \) problem size
- Example: Power lookup table:

<table>
<thead>
<tr>
<th>( g )</th>
<th>( m )</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>745</td>
<td>1</td>
<td>89.79</td>
<td>169.91</td>
<td>314.53</td>
<td>550.91</td>
</tr>
<tr>
<td>810</td>
<td>93.51</td>
<td>176.05</td>
<td>324.59</td>
<td>567.11</td>
<td></td>
</tr>
<tr>
<td>875</td>
<td>98.80</td>
<td>185.46</td>
<td>341.26</td>
<td>589.41</td>
<td></td>
</tr>
</tbody>
</table>
**Prediction Error**

**Performance**
- Prediction error is within 5% for 99% of the tests

**Power**
- Prediction error is within 10% for 99% of the tests

---

**Summary of CPU and GPU experiments**

- The following assumptions are experimentally verified
  - Performance at lower clock frequencies may be derived from the performance of the application at the highest clock frequency holds both for CPUs and GPUs
  - Power consumption does not depend on problem size holds for both CPUs and GPUs
- The above assumptions help to reduce the number of required experiments further
## Hybrid Experiments

### Parameters Values

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Load ((x, y))</td>
<td>((1024, 7168), (1152, 6912), (1280, 6784), (1380, 6656), (1480, 6528), (1592, 6396), (1664, 6272), (1792, 6144), (1920, 6016), (2048, 5888), (2176, 5760), (2304, 5632), (2432, 5504), (2560, 5376), (2688, 5248), (2816, 5120), (2944, 4992), (3072, 4864), (3200, 4736), (3328, 4608), (3456, 4480))</td>
</tr>
<tr>
<td>(x)</td>
<td>CPU load</td>
</tr>
<tr>
<td>(y)</td>
<td>GPU load</td>
</tr>
<tr>
<td>(f)</td>
<td>(1200, 1500, 1800, 2100, 2400)</td>
</tr>
<tr>
<td>(g)</td>
<td>(745, 810, 875)</td>
</tr>
<tr>
<td>(n)</td>
<td>(2, 4, 8, 12)</td>
</tr>
<tr>
<td>(m)</td>
<td>(1, 2, 4, 8)</td>
</tr>
</tbody>
</table>

### Hybrid Experiments

<table>
<thead>
<tr>
<th>CPU</th>
<th>GPU</th>
<th>Predicted Energy (J)</th>
<th>Actual Energy (J)</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>elements</td>
<td>count</td>
<td>GHz</td>
<td>elements</td>
<td>count</td>
</tr>
<tr>
<td>2540</td>
<td>8</td>
<td>2.4</td>
<td>5652</td>
<td>2</td>
</tr>
<tr>
<td>2621</td>
<td>8</td>
<td>2.4</td>
<td>5571</td>
<td>2</td>
</tr>
<tr>
<td>2621</td>
<td>8</td>
<td>2.4</td>
<td>5571</td>
<td>2</td>
</tr>
<tr>
<td>2540</td>
<td>8</td>
<td>2.4</td>
<td>5652</td>
<td>2</td>
</tr>
<tr>
<td>2293</td>
<td>8</td>
<td>2.4</td>
<td>5899</td>
<td>2</td>
</tr>
<tr>
<td>1474</td>
<td>4</td>
<td>2.4</td>
<td>6718</td>
<td>2</td>
</tr>
</tbody>
</table>

- Error in prediction for some of the best predicted configurations for minimum energy consumption
Hybrid Experiments

- Energy versus performance pareto optimal curve. Red line shows the predicted curve, while blue line is obtained from actual data.

Pareto Curves for Energy Versus Runtime

- Data for each Pareto-optimal point contain the following information in order: CPU load (%), CPU count, GPU count, CPU frequency (GHz), GPU frequency (MHz), energy (J), time (s).
Multi-Level Memories

KNL Overview

- Running time is total time taken to complete 100 time steps
- Optimizations on KNL include autotuning, vectorization AVX-512 instructions, using OpenMP + MPI, using MCDRAM as cache

CMT-bone on Intel KNL

Running time is total time taken to complete 100 time steps
Optimizations on KNL include autotuning, vectorization AVX-512 instructions, using OpenMP + MPI, using MCDRAM as cache
CCMT

**CMT-bone on Different Platforms**

- KNL is faster than an Intel IvyBridge by about 4 times
- KNL is faster than Tesla K40m GPU by about 3 times
- KNL is the most energy efficient platform

![Graph showing running time in seconds for different platforms.](image)

**TDP: 150W**

**TDP: 245W**

**TDP: 215W**

---

**Publications**

Conclusions: Overall Improvement

Performance per Watt Improvement

Algorithmic

Hardware

Dynamic Voltage Scaling
Dynamic Load Balancing
Multi-Level Memories
Energy Tradeoffs
Hybrid Core
Mapping

Overall Improvement \( X^* Y \)

Do you have any questions?

Particle Elements

Xeon
K40
KNL

TDP: 150W
TDP: 245W
TDP: 215W
CPU Experiments

- Constant of proportionality, for total execution time

<table>
<thead>
<tr>
<th>f</th>
<th>n</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>0.975</td>
<td>0.965</td>
<td>0.965</td>
<td>0.935</td>
<td>0.905</td>
<td></td>
</tr>
<tr>
<td>1500</td>
<td>0.985</td>
<td>0.985</td>
<td>0.975</td>
<td>0.955</td>
<td>0.915</td>
<td></td>
</tr>
<tr>
<td>1800</td>
<td>0.995</td>
<td>0.995</td>
<td>0.990</td>
<td>0.985</td>
<td>0.975</td>
<td></td>
</tr>
<tr>
<td>2100</td>
<td>0.990</td>
<td>0.990</td>
<td>0.990</td>
<td>0.990</td>
<td>0.970</td>
<td></td>
</tr>
</tbody>
</table>

- Constant of proportionality, for communication time

<table>
<thead>
<tr>
<th>f</th>
<th>n</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>0.82</td>
<td>0.88</td>
<td>0.82</td>
<td>0.72</td>
<td>0.62</td>
<td></td>
</tr>
<tr>
<td>1500</td>
<td>0.86</td>
<td>0.86</td>
<td>0.86</td>
<td>0.77</td>
<td>0.70</td>
<td></td>
</tr>
<tr>
<td>1800</td>
<td>0.90</td>
<td>0.90</td>
<td>0.90</td>
<td>0.83</td>
<td>0.80</td>
<td></td>
</tr>
<tr>
<td>2100</td>
<td>0.95</td>
<td>0.95</td>
<td>0.95</td>
<td>0.92</td>
<td>0.90</td>
<td></td>
</tr>
</tbody>
</table>

Hardware-Software Autotuning

Algorithm: dudr-4loop
\[
\text{do } k = 1, N_z \\
\text{do } j = 1, N_y \\
\text{do } i = 1, N_x \\
\text{do } l = 1, N_x \\
\quad dudr(I, j, k) = dudr(I, j, k) + a(i, l) * u(l, j, k, ie) \\
\text{enddo} \\
\text{enddo} \\
\text{enddo} \\
\text{enddo}
\]

Algorithm: dudr-4loop-fused
\[
\text{do } k = 1, N_z * N_y \\
\text{do } i = 1, N_x \\
\text{do } l = 1, N_x \\
\quad dudr(k, i) = dudr(k, i) + a(i, l) * u(l, k, ie) \\
\text{enddo} \\
\text{enddo} \\
\text{enddo}
\]

Algorithm: dudr-4loop-permuted-and unrolled
\[
\text{do } k = 1, N_z \\
\text{do } j = 1, N_y \\
\text{do } i = 1, N_x \\
\text{do } l = 1, N_x \\
\quad dudr(j, k) = dudr(j, k) + a(i, l) * u(l, j, k, ie) \\
\quad dudr(j+1, k) = dudr(j+1, k) + a(i, l+1) * u(l+1, j, k, ie) \\n\text{enddo} \\
\text{enddo} \\
\text{enddo} \\
\text{enddo}
\]

Number of 4-loop implementations for dudr
\[N_x = N_y = N_z = 10\]
\[= 4! * 4^4\]
\[= 24 * 256 = 6144\text{ variants}\]
Total number of variants = 98,240 (N=10)
Total number of variants = 217,728 (N=20)
Exhaustive search may not be feasible
**Genetic Algorithm**

- Compile and run each individual
- Set fitness value for each individual based on performance and energy
- Generate Initial Population
- Population Selection
- Add new individuals using crossover and mutation
- $i = i+1$

**Comparison of GA with Exhaustive Approach**

### Comparison of performance by platform

<table>
<thead>
<tr>
<th>Platforms</th>
<th>CMT- nek time (seconds)</th>
<th>Exhaustive Autotuning</th>
<th>GA based Autotuning</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time</td>
<td>Search Space</td>
<td>% Less</td>
</tr>
<tr>
<td>IBM BG/Q</td>
<td>5.57</td>
<td>2.54</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Opteron</td>
<td>1.81</td>
<td>1.02</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Fusion</td>
<td>1.36</td>
<td>0.95</td>
<td>9771</td>
</tr>
</tbody>
</table>

### Comparison of energy consumption by platform

<table>
<thead>
<tr>
<th>Platforms</th>
<th>CMT- nek energy (Joules)</th>
<th>Exhaustive Autotuning</th>
<th>GA based Autotuning</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Energy</td>
<td>Search Space</td>
<td>% Less</td>
</tr>
<tr>
<td>IBM BG/Q</td>
<td>292.1</td>
<td>131.7</td>
<td>9771</td>
</tr>
<tr>
<td>AMD Fusion</td>
<td>17.6</td>
<td>11.98</td>
<td>9771</td>
</tr>
</tbody>
</table>

Results (AMD Fusion @ Sandia)
Performance (varying hardware parameters)

Best Time (seconds)

Line Size -
Associativity

Cache size

Associativity Tuning

GEM5 environment

Instruction set architecture: X86
CPU model: Out-of-order CPU
Memory model: Classic, DDR3
Clock frequency: 1GHz

Capacity Tuning

Line Size Tuning

Power for most configurations is nearly the same. Thus, energy requirements are similar.

Genetic Algorithm based Autotuning Approach for Performance and Energy Optimization, Tania Banerjee and Sanjay Ranka (SUSCOM, to appear)
Exascale Behavioral Emulation

Principal Investigators:

Herman Lam, Greg Stitt
Center for Compressible Multiphase Turbulence (CCMT)
NSF Center for High-Performance Reconfigurable Computing (CHREC)
ECE Department, University of Florida

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FPGA Acceleration

Sai Chenna
BE Design Space Exp.

Trokon Johnson
BE Tools

Aravind Neelakantan
BE Methods

Nalini Kumar
BE Methods

Carlo Pascoe
FPGA Acceleration

Raj Rajagoplan
BE-SST

Ben Reynolds
Thermal Modeling

Chad Saunders
FPGA Acceleration
Outline

- Review & overview:
  - Behavioral Emulation (BE)

Research thrusts & achievements

- BE-SST simulator & tools, experimental results
- BE method enhancements
  - Multi-fidelity surrogate model for performance prediction
  - Symbolic regression for performance modeling
  - Thermal experiments & modeling
- CMT-nek design space exploration using BE simulation
- Acceleration using FPGAs
  - Of BE: speedup vs BE-SST, scale up on multiple FPGAs
  - Of CMT-nek kernels: approach & preliminary results

- Summary, conclusions, & future work
Co-Design Using Behavioral Emulation

**HW/SW co-design**
- Algorithmic & architectural design-space exploration (DSE)

**Coarse-grained BE simulation**
- Balance of simulation speed & accuracy for rapid design-space evaluation

Outline

- Review & Overview:
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Research thrusts & achievements

- **BE-SST simulator & tools**, experimental results
- BE method enhancements
  - Multi-fidelity
  - Symbolic
  - Thermal
- CMT-nek design space exploration
- Acceleration
  - Of BE: symbolic
  - Of CMT-nek

- Summary, conclusions, & future work
BE-SST Simulator*

- Developed by extending Structural Simulation Toolkit (SST)**
  - Framework for parallel simulations
  - Supported by developers & vendors
  - Flexibility in designing custom components


BE-SST Enhancements

- Developed interpolation API
  - To select appropriate interpolation techniques (e.g., Linear interpolation, polynomial interpolation)
- Since AST review 2017: support for symbolic regression
  - Improve accuracy (More details later)
- Able to support trace-driven simulation*
  - For time-dependent simulations
  - To mimic CMT-nek with particles more accurately
- Inclusion of collective-communication operations
  - MPI_ISEND, MPI_Irecv, MPI_WAITALL
- Communication model
  - Replaced static routing method with dynamic routing
- Leverage parallel capabilities of SST for BE-SST

* More details in Sai Chenna’s presentation on Tuesday
**Dynamic Routing**

- Replaced static routing method with dynamic routing
  - Improve BE-SST scaling: large static routing table not required for increasing number of cores (Fig. 1)
  - Build-time benefits: Config build time not a bottleneck for large simulation (Fig. 2)

**Parallel Performance of BE-SST**

- Simulations of Vulcan System with 5-D Torus Topology*
  - 4K, 32K, 128K core
- Improved parallel performance with increase in problem size
  - For e.g., 128k core simulation
    - Without parallelization (1 rank): ~1 day;
    - With 256-rank parallelization: 17 min.

* Run using BE-SST installed on Titan
**BE-SST Scalability**

- Aiming for 1M+ cores; able to simulate 800K+
  - Memory bottleneck
- Uneven memory distribution across ranks while simulating
  - Bigger systems (e.g., 1 Million+ cores)
  - With more complex interconnects (e.g., 5D Torus of Vulcan)

* GCM
Graph Construction Memory: initial memory allocation before simulation

- Working with Sandia National Labs (Jeremy Wilke) to solve this issue

---

**Outline**

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    - Symbolic
    - Thermal
  - CMT-nek design space exploration using BE simulation
  - Acceleration
    - Of BE itself
    - Of CMT-nek

- Summary, conclusions, & future work
BE simulations of HPC systems

- **Titan @ ORNL**
  - Cray XK7 architecture with Cray Gemini interconnect
  - 16-core AMD opterons; 18k nodes; 300k cores
  - 18k K20X Kepler GPUs
  - 32GB + 6GB memory/node

- **Vulcan @ LLNL**
  - IBM BG/Q architecture
  - 16 cores/node, 24k nodes, 390k cores
  - 16GB memory/node

Application Case Study: **CMT-bone-BE**

- CMT-nek & CMT-bone (mini-app) both are large codes
- To support extensive DSE*, we need:
  - Key compute kernels & comm. patterns that affect performance
  - Abstract, modular, easy to modify and instrument for algorithmic DSE

- Computation- & communication-intensive portions of CMT-nek workflow in C & MPI
  - Volume-to-surface data extraction
  - Face data exchange (with neighbors)
  - Derivative computation volume points
- Easier to modify for algorithmic DSE
- 1000 vs 10s of thousands lines of code

* design-space exploration
Experiment Setup

- Application case study: CMT-bone-BE (gas solver)
- Application parameters
  - Calibration
    - element size: 5,9,13,17,21
    - elements/core: 8,32,64,128,256
  - Validation
    - element size: 5,6,9,11,16,17
    - 64 elements/core
- Machine parameters
  - Validation up to 128k MPI ranks
  - Predictions up to 1M MPI ranks
  - Can perform both predictions and validations for larger systems
- Monte-Carlo Simulations

BE Simulations of CMT-bone-BE on Titan+

- Simulating bigger system than Titan (up to 1 Million cores)
- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 17%

\[
\% \text{ error} = \frac{N \sum_{i=1}^{N} |\text{measured}_i - \text{predicted}_i|}{N} \times 100
\]
Simulating a bigger system than Vulcan (512k cores)
- Average % error between CMT-bone-BE simulation and execution time is 4%
- Maximum error is 9%

Notional architecture
- IBM POWER architecture
- 48 cores/node
- Non-blocking fat-tree topology
- Tending towards Summit @ ORNL

Initial methodology
- OSU n/w benchmark* of Cab (fat-tree topology)
- Lookup tables of Vulcan (POWER architecture)
- Predictions up to 128k MPI ranks

*developed in Ohio State University
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  - Symbolic regression for performance modeling
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- Acceleration
  - Of BE: sp
  - Of CMT-nek: ...

- Summary, conclusions, & future work

Behavioral Emulation with UQ

Goal: Improve BE models via validation and uncertainty estimation

- Reduce computational budget by fitting BE simulation to CMT-nek using Multi-Fidelity Surrogate (MFS)
- Extrapolation of CMT-nek towards large-scale runs using BE and MFS
Multi-fidelity Prediction of CMT-nek

Experimental setup

- Design of experiment (DOE)
  - Element size (ES) = 5, 9, 13, 17, 21
  - Elements per processor (EPP) = 8, 32, 64, 128, 256
  - Number of processors (NP) = 16, 256, 2048, 16384, 131072

- 125 total data points
  - BE simulation: all 125 runs
  - CMT-nek: 22 runs
  - CMT-bone: 67 runs

- Multi-fidelity surrogate model
  - Fitting CMT-nek using corrected fitting of BE simulation
  - For large problems, low-fidelity BE simulation is computationally cheaper than high-fidelity CMT-nek or CMT-bone

Accuracy of corrected BE sim.

- At 10 left-out CMT-nek test points
- Overall RMSE < 10% with 7 or more CMT-nek data
- Reducing computation budget
  - Supplementing high-fid. (CMT-nek) with low-fid. (BE simulation) runs

Extrapolation Towards Large-scale Runs

- Extrapolation necessary for exascale prediction
  - But challenging due to limited runs
- Develop MFS using:
  - 7 (out of 22) runs of CMT-nek (high-fidelity), at 256 and 2k processors
  - All 125 BE simulations (low-fidelity)
- Extrapolate using MFS towards 16k (11 runs) & 128k (4 runs) processors

Extrapolation: Validation

- Extrapolate using MFS towards 16k (11 runs) and 128k (4 runs) processors
  - Linear fit to CMT-nek: poor result
    - High-order fitting leads to overfitting due to limited samples (7 CMT-nek runs with 3 variables)
  - MFS: relative errors less than 11%
Extrapolation: Prediction of CMT-nek

- MFS prediction towards one million processors with UQ
  - 64 elements per processors (9 CMT-nek runs)
  - MFS predictions
- Monotonic trend with small curvature in logarithmic coordinate

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    - Thermal
  - CMT-nek
  - Acceleration
    - Of BE
    - Of CMT-nek
- Summary
Symbolic Regression: Motivation

- Motivation:
  - Multi-parameter performance modeling is challenging
  - Requires accuracy, computational efficiency, simple implementation

- Our previous approaches:
  - N-dimensional interpolation:
    - Computationally expensive
    - Difficult to implement, needs customization for each example
    - Insufficient accuracy
  - Multi-variate linear regression:
    - Faster than interpolation, relatively simple to implement
    - Need thorough understanding of code to generate performance models
    - May not capture machine-specific behaviors that deviate from basic model

Symbolic Regression

- Advantages:
  - Captures machine-specific performance behaviors
  - Enables tradeoffs between accuracy and computational complexity
    - Can maximize performance for a given error constraint
  - Requires no prior knowledge of the kernel

- Approach: custom genetic-programming tool
  - Evolves “trees” from mathematical primitives
  - Multiple optimization goals: minimize error, minimize error given tree size constraint, minimize tree size given error constraint, etc.
### Symbolic Regression: Results

<table>
<thead>
<tr>
<th>Particle solver kernel</th>
<th>Linear Regression</th>
<th>Symbolic Regression</th>
<th>Error Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RMSE</td>
<td>MAPE</td>
<td>RMSE</td>
</tr>
<tr>
<td>Compute1</td>
<td>4.43E-06</td>
<td>3.5%</td>
<td>1.08E-05</td>
</tr>
<tr>
<td>update_particle_location</td>
<td>1.26E-05</td>
<td>10.8%</td>
<td>1.26E-05</td>
</tr>
<tr>
<td>particles_in_grid</td>
<td>1.17E-02</td>
<td>76.4%</td>
<td>1.27E-02</td>
</tr>
<tr>
<td>interp_props_part_location</td>
<td>4.51E-01</td>
<td>902.6%</td>
<td>3.67E-01</td>
</tr>
<tr>
<td>upd_vel_and_pos_rk3_stage1</td>
<td>8.22E-04</td>
<td>399.0%</td>
<td>5.43E-04</td>
</tr>
<tr>
<td>upd_vel_and_pos_rk3_stage3</td>
<td>1.06E-04</td>
<td>19.4%</td>
<td>6.50E-05</td>
</tr>
<tr>
<td>upd_vel_and_pos_rk3_allstage</td>
<td>7.34E-03</td>
<td>27.3%</td>
<td>7.57E-04</td>
</tr>
<tr>
<td>upd_vel_and_pos_bclf</td>
<td>5.38E-04</td>
<td>20.0%</td>
<td>1.21E-03</td>
</tr>
<tr>
<td>red_interp</td>
<td>9.33E-02</td>
<td>4.7%</td>
<td>2.94E-02</td>
</tr>
<tr>
<td>user_particles_forces</td>
<td>8.80E-05</td>
<td>6.3%</td>
<td>6.85E-05</td>
</tr>
<tr>
<td>tri_interp</td>
<td>1.58E-04</td>
<td>1.4%</td>
<td>5.34E-05</td>
</tr>
<tr>
<td>Average</td>
<td>5.14E-02</td>
<td>133.8%</td>
<td>3.75E-02</td>
</tr>
</tbody>
</table>

---

### Outline

- **Review & Overview:**
  - Behavioral Emulation (BE)
- **Research thrusts & achievements**
  - BE-SST simulator & tools, experimental results
  - BE method enhancements
    - Multi-fidelity surrogate model for performance prediction
    - Symbolic regression for performance modeling
    - Thermal experiments & modeling
  - CMT-nek design space exploration using BE simulation
  - Acceleration using FPGAs
    - Of BE: speedup vs BE-SST, scale up on multiple FPGAs
    - Of CMT-nek kernels: approach & preliminary results
- **Summary, conclusions, & future work**
Thermal Benchmarking & Modeling

- Previously modeled energy/power using physical and simulation measurements
- Current focus: thermal modeling with IR images of KNL
  - Goal: minimize maximum temperature via load balancing
- More challenging than anticipated
  - CPU fans block thermal information of CPU
  - Tried custom fan setup, destroyed several processors
- Modified KNL for IR by cutting hole in case:

Observations:
- Heat sink “blocks” much of processor
- Minimizing the maximum temperature may not be most appropriate optimization goal
- Future work: investigate how heat changes for different load balancing optimizations
  - Determine most approach optimization goal
Outline

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- Summary, conclusions, & future work

CMT-nek DSE: Motivation & Approach

- Motivation:
  - CMT-nek has huge design space
  - Various architectural options exist for Exascale systems

- Goal:
  - Use BE methods & tools to perform DSE

- Approach: Iterative DSE steps
  - Perform BE Simulations of CMT-nek (baseline)
  - Identify optimization candidates (i.e. most expensive subroutines)
  - Create and validate models of algorithms for these subroutines
  - Use BE to predict performance
BE-SST Predictions: Particle solver

- **Summary of results**
  - **Interpolation:**
    - scales non-linearly w.r.t element size and elements-per-processor, linearly w.r.t particles/gridpoint
    - Reduced barycentric is 5x faster than barycentric interpolation
    - Trilinear interpolation is on average 164x faster than barycentric interpolation
  - **Time integration:**
    - scales non-linearly w.r.t element size and elements-per-processor, linearly w.r.t particles/gridpoint
    - Bdf is 3x faster than rk3 time integration

- **Refer to Sai Chenna’s presentation**
  - BE Simulations of CMT-nek

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BE Design-Space Exploration

Example design space:
- 20 values for lelt, lx1, lpart
- 10 different numbers of cores
- 10 different core types
- 10 different memory configurations
- 4 different network topologies

32 million options to explore

- **BE Advantage**: significantly faster than existing simulators
- **BE Limitation**: still not fast enough for DSE of exascale systems
- **Approach**: Use FPGA acceleration to improve exploration
  - Sacrifice analysis capabilities to prune design space
  - Use BE-SST to analyze remaining candidates

---

**Fully-expanded Pipeline (FEP)**

1. Construct Data Flow Graph (DFG) from simulation configuration
   - AppBEO+ArchBEO define instructions and operand/output dependencies
   - Instructions map to vertices and dependencies map to edges in DFG
   - Various opportunities for graph-level optimizations

2. Map DFG to pipeline circuit
   - Vertex attributes define operations and instantiate dedicated HW
   - Edge attributes (e.g., src/dst) instantiate pipeline register between src/dst pair
   - Various opportunities for circuit-level optimizations

Because each instruction (from sim) mapped to independent HW (no resource sharing), each vertex able to start next sim 1 cycle after current sim
**Collapsed Pipeline (CP)**

1. Construct Data Flow Graph (DFG) from simulation configuration
   - AppBEO+ArchBEO define instructions and operand/output dependencies
   - Instructions map to vertices and dependencies map to edges in DFG
   - Partition into linear subgraphs and generate dependency lists

2. Mapping DFG to FPGA Pipeline
   - Vertex attributes define operations and
   - Edge attributes instantiate pipeline register between src/dst pairs
   - Align subgraph traces such that cost is minimized and no dependencies are violated

Because each subgraph instruction mapped to independent HW, each vertex able to start next subgraph 1 cycle after current subgraph. All subgraphs must complete before sim can complete.

**Fully-Expanded & Collapsed Pipeline Tradeoffs**

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>Num. of Events</th>
<th>% LU</th>
<th>Latency Hardware</th>
<th>Hardware</th>
<th>RE-SST</th>
<th>Hardware Speedup</th>
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<td>300/3.5</td>
<td>12,128/120.6</td>
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**Fully-Expanded Pipeline**

Advantages:
- Superior performance in terms of simulation throughput and latency
- 280-320 MHz implies 280-320 million simulations per second independent of simulated MPI ranks

Limitations:
- Resources scale linearly with both MPI Ranks and number of timesteps
- Scaling across multiple FPGAs expected to be ineffective when considering exascale simulations
### Fully-Expanded & Collapsed Pipeline Tradeoffs

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>Num. of Events</th>
<th>% LU</th>
<th>Latency (cycles)</th>
<th>Hardware MSPS†</th>
<th>Hardware GEPS‡</th>
<th>BE-SST KEPSP</th>
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<td>10.5</td>
<td>27,712</td>
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</tbody>
</table>

†Mega-Simulations-Per-Second, ‡Giga/Kila-Events-Per-Second, ‘–’ indicates configuration unable to fit on a single FPGA

---

### Collapsed Pipeline Single-FPGA Performance/Scalability

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>Num. of Events</th>
<th>% LU</th>
<th>Latency (cycles)</th>
<th>Hardware MSPS†</th>
<th>Hardware GEPS‡</th>
<th>BE-SST KEPSP</th>
<th>Hardware Speedup</th>
</tr>
</thead>
<tbody>
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<td>460</td>
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<td>19x</td>
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<td>551</td>
<td>2.17</td>
<td>25x</td>
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<tr>
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<td>3.10x†</td>
<td>X</td>
<td>X</td>
<td>X</td>
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</table>

As number of ranks increase:
- additional logic per rank approaches zero
- simulation throughput reduced by a factor of “ranks”
- event throughput remains proportional to instantiated event hardware

### Advantages:
- Resources scale linearly with timesteps, but sublinearly with MPI Ranks
- allows for significantly more timesteps due to its much lower base utilization
- Better scaling on single and multiple FPGAs

### Limitations:
- Lower simulation throughput and longer initial latency, but still more than sufficient for rapid design-space exploration

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### Now able to reach million+ rank simulations in hardware

- Rank limit due to insufficient blockram not logic
- Expect greater performance when Stratix 10 becomes available

**Throughput > 10Mx higher than BE-SST**

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### Increased performance expected with Stratix 10
- Collapsed hardware specifically designed to exploit new Stratix 10 architecture

---

**Center for Compressible Multiphase Turbulence**

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Pipelines scale linearly with the length of simulation, but as a single, unidirectional pipe

— Partitioned easily/predictably across any number of connected FPGAs

Given a desired # of simulated ranks, timesteps, granularity (events per timestep), we can predict performance & # of FPGAs

Main point: FPGAs achieve similar scale as BE-SST, but orders of magnitude faster

— 1M ranks, 300+ of sims/second

<table>
<thead>
<tr>
<th>Ranks</th>
<th>TS</th>
<th>FPGAs</th>
<th>Num. of Events</th>
<th>Lat to First Out (cycles)*</th>
<th>Mega Sims /second*</th>
<th>Giga Events /second*</th>
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</table>

Novo-G#

• 64 GIDEL ProceV (Stratix V)
• 4x4x2 3D torus or 5D hypercube
• 6 Rx-Tx links per FPGA
• Measured 32 Gbps per link
• 150 ns latency across links
• Require 64bits/cycle between FPGAs
• 335MHz, 21.4 Gbps, 51 additional lat
• 450MHz, 28.8 Gbps, 68 additional lat
• 500 MHz before link BW saturation

**FPGA Acceleration Trends**

- **FPGAs growing trend in data centers**
  - Microsoft Catapult, Amazon F1, Intel Broadwell+FPGA
  - National lab interest

- **Recently performed case study**
  - on Intel Broadwell+Arria 10 (BDW+A10) for 2D convolution
  - 96x less energy than Broadwell
  - 15.7x less energy than P6000 GPU

- **Future research?**
  - FPGA acceleration of CMK-nek functions

---

### Energy Comparison of BDW+A10 vs. Broadwell

<table>
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<tr>
<th>Precision</th>
<th>Kernel Size</th>
<th>768x256</th>
<th>512x512</th>
<th>256x1024</th>
<th>2048x1024</th>
<th>Avg</th>
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<tbody>
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<td>16x</td>
<td>67x</td>
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<tr>
<td>7x7</td>
<td>58x</td>
<td>135x</td>
<td>133x</td>
<td>164x</td>
<td>128x</td>
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<tr>
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<td>138x</td>
<td>136x</td>
<td>148x</td>
<td>106x</td>
<td></td>
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<tr>
<td>Avg</td>
<td>51x</td>
<td>99x</td>
<td>131x</td>
<td>140x</td>
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</tbody>
</table>

**Energy Comparison of BDW+A10 vs. P6000 GPU**

<table>
<thead>
<tr>
<th>Precision</th>
<th>Kernel Size</th>
<th>768x256</th>
<th>512x512</th>
<th>256x1024</th>
<th>2048x1024</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>16-bit Fixed 3x3</td>
<td>5x5</td>
<td>15.5x</td>
<td>19.8x</td>
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<td>19.0x</td>
<td>18.4x</td>
</tr>
<tr>
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<td>10.5x</td>
<td>18.2x</td>
<td>19.7x</td>
<td>20.5x</td>
<td>17.2x</td>
<td></td>
</tr>
<tr>
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<td>15.3x</td>
<td>16.9x</td>
<td>18.6x</td>
<td>14.7x</td>
<td></td>
</tr>
<tr>
<td>Avg</td>
<td>11.8x</td>
<td>18.0x</td>
<td>18.9x</td>
<td>19.5x</td>
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<td></td>
</tr>
</tbody>
</table>

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**Summary & Conclusions**

- **BE methods & tools**
  - **BE method enhancements**: network models, interpolation & symbolic regression schemes, energy & thermal modeling
  - **BE-SST enhancements**: functionality, tools, & scaling

- **Large-scale experiments**
  - Validation (100k+ MPI ranks) on Titan & Vulcan
  - Predictive simulations to million+ MPI ranks; on notional archs

- **CMT-nek DSE using BE simulation**
  - Profiling of key CMT-nek particle solver routines
  - Accuracy/performance tradeoffs using BE simulation

- **FPGA acceleration of BE simulation**
  - Validation of dataflow, pipelined approaches (FEP, CP)
  - multi-FPGA scalability prediction & validation
Do you have any questions?